Understanding metallic bonding:

Structure, process and interaction by Rasch analysis

Abstract

This paper reports the results of a survey of 3,006 Year 10-12 students on their understandings of metallic bonding. The instrument was developed based on Chi's ontological categories of scientific concepts and students' understanding of metallic bonding as reported in the literature. The instrument has two parts. Part one probes into students' understanding of metallic bonding as (a) a submicro *structure* of metals, (b) a *process* in which individual metal atoms lose their outermost shell electrons to form an sea-electron and octet metal cations, or (c) an all-directional electrostatic force between delocalized electrons and metal cations, that is, an *interaction*. Part two assesses students' explanation of malleability of metals, for example (a) as a submicro structural rearrangement of metal atoms/cations or (b) based on all-directional electrostatic force. The instrument was validated by the Rasch Model. Psychometric assessment showed that the instrument possessed reasonably good properties of measurement. Results revealed that it was reliable and valid for measuring students' understanding of metallic bonding. Analysis revealed that the *structure*, *process* and *interaction* understandings were unidimensional and in an increasing order of difficulty. Implications for the teaching of metallic bonding, particular through the use of diagrams, critiques and model-based learning, are discussed.

Keywords: conceptual change, ontological categories, model-based learning

Introduction

Two Models of Metals in School Chemistry

Learning of school science can be regarded as a progressive study of different models of physical phenomena (Gilbert, 2004; Schwarz et al., 2009). The same physical phenomena could be represented by different models with different levels of sophistication at different levels of study. It is likely students' understanding of a more advanced model is informed by their earlier learning. This study investigated different ways in which senior secondary students might understand the free electron model of metals.

In junior secondary (Years 7-9), students in Hong Kong and in many countries are introduced to general ideas of the particulate nature of matter, or the simple particle model (Tsaparlis & Sevian, 2013). Metals are considered as being made up of particles, with each metal made of one kind of particles. The change of states as a macroscopic phenomenon is ascribed to different spatial arrangements of metal particles in different states. Nevertheless, the attraction between particles is not considered at this level. Rather, the focus of this model at the Years 7-9 level is the submicro representations of metal structure.

In senior secondary (Year 10 or above), students are introduced to the idea that metals are composed of a lattice of metal cations where there are delocalized electrons moving around them. This model may be called the free electron model of metals. The learning at this level focuses on not only the submicro structure that is made of metal cations and delocalized electrons, but also the all-directional electrostatic force, known as metallic bonding, between these structural constituents. Previous studies have suggested that students face many challenges in learning this model (de Posada, 1997; Taber, 2003b; Coll & Treagust, 2003). In an interview study, Cheng and Gilbert (2014) postulated that the learning was challenging because it involved a conceptual change from the focus on structure (in the

simple particle model) to a focus on the intangible electrostatic force also (in the free electron model). We sought to extend their work by examining a larger population of students to determine whether learning the electrostatic force was more challenging than learning it as a structure.

An understanding of the free electron model must involve not only its description, but also what it can explain that the simple particle model cannot (Hadenfeldt, Liu, & Neumann, 2014). For example, both models explain the malleability of metals, but at different levels of precision. The simple particle model explains it as the spatial rearrangement of particles before and after a metal is stressed. Nevertheless, it does not explain why metals specifically possess such a property that is not shared by ionic and covalent substances. The free electron model suggests that when a metal is being stressed, the free electrons can still hold the metal cations through the all-directional electrostatic force. As ionic or covalent substances have different structural constituents, although some of them can be very strong, they are not malleable. We noted that learning a model involves its description and its explanations of phenomena (Treagust, Chittleborough, & Mamiala, 2002; Karpin, Juuti, & Lavonen, 2014). Therefore, when we surveyed students' understanding of metallic bonding, we asked the students to both describe it and state how it explained the malleability of metals.

Conceptual Change in Learning the Free Electron Model

This study was informed by the idea that some scientific concepts can be classified into different ontological categories, namely, 'entities' or 'processes' (Chi, Slotta, & De Leeuw, 1994; Chi, 2013). Learning a new concept can be especially challenging when it belongs to an ontological category that differs from students' preconceptions. Chi (2013) proposed that the

learning of forces in Newtonian mechanics involved a shift from students' prior understanding of a force as an 'entity' (that can be shared or used up) to the scientific idea of forces as interactions between two objects, which she called a 'process' or an 'emergent process'.

The previous section suggests that the simple particle model focuses on the spatial structure of particles in different states of metals (i.e., entity); the free electron model focuses on the electrostatic force between each delocalized electron and metal cation (i.e., emergent process, according to Chi). The learning of the free electron model of metallic bonding based on the existing knowledge of the simple particle model arguably involves an ontological shift. It has been shown that such a shift might present a big challenge to students (Cheng & Gilbert, 2014).

Based on previous studies and our observation of some official assessment guides, an understanding of metallic bonding may fall into the following categories.

(1) Bonding was regarded as a structure (or an 'entity' according to Chi (2013)). In this case, metal cations and delocalized electrons *per se* were considered metallic bonding. In this paper, *structure* (italicized) is used to denote this category of understanding.

(2) Bonding was regarded as a process, or involved a process, in which atoms attain octet and/or form a sea of electrons (Assessment and Qualifications Alliance (AQA), 2010, 2012). According to Chi, this is a 'sequential process'. In this paper, *process* (italicized) is used to denote this category of understanding. It has also been reported that students considered bonding as a process in which electrons are shared, gained or lost (Taber, 2001; Taber, Tsaparlis, & Nakiboğlu, 2012; Nahum, Mamlok-Naaman, Hofstein, & Taber, 2010). This category of understanding is different from *structure* and is not an electrostatic force. However, the *process* understanding of chemical bonding has been prevalent among some students and has even been suggested in curriculum documents.

Also, some students could describe the sequential process of forming the electron sea without indicating the electrostatic force between electrons and cations (Cheng & Gilbert, 2014). It is thus important that such a category of understanding be conceptualized as a possible student understanding.

(3) Bonding was regarded as the electrostatic force between delocalized electrons and metal cations. We suggest that metallic bonding also shares features of emergent processes (based on Chi, 2013, p.65, Table 3.2). In sequential processes, the agents of a system behave in distinct ways and sequentially. As a *process*, metal atoms lose the outermost shell electrons and form an electron sea and an octet structure. It is the atoms that lose electrons (but not the other way around), and metal atoms become metal ions and an electron sea (but not in a reverse sequence). In emergent processes, all of the agents behave in a more or less uniform way simultaneously; there is an electrostatic attraction between each electron and each metal cation reciprocally and simultaneously. Such an understanding is key to metallic bonding and to explaining the malleability of metals. In this paper, we use *interaction* (italicized) as shorthand for the emergent process as a category of understanding. The label makes it more explicit and direct that bonding is a force between two objects, namely, delocalized electrons and metal cations.

In short, the preceding discussion highlights three distinctive categories of understanding. This study tested whether *structure*, *process* and *interaction* could be considered as types of understanding with different levels of difficulty. The findings of this study can be used to empirically test Chi's theory of ontological categories and more specifically to make sense of students' learning of metallic bonding. In the next section, we discuss the assumption behind our suggestion that the *interaction* understanding is of the highest level, followed by *process* and *structure* understanding.

We suggest that the *interaction* understanding is at the highest level. The reasons are as follows.

(1) **Interaction *is based on* structure.** Metallic bonding is the electrostatic force between metal cations and delocalized electrons. The force is an intangible interaction between the two structural entities of metals at the submicro level. A scientific understanding of metallic bonding must be based on the spatial structure of metal cations and delocalized electrons. Yet, an accurate recall of the structure did not guarantee a scientific understanding of the *interaction* between the structural constituents (Cheng & Gilbert, 2014).

(2) **Interaction *offers more precise explanations of properties*.** The simple particle model (taught in Years 7-9) focuses on the different structural arrangements of particles in different physical states, and stresses that particles are not destroyed in any physical or chemical changes. In other words, the focus is on the *structure* category of understanding. Explanations for characteristic physical properties of metals are beyond the reach of the simple particle model. From Year 10 onwards, students are expected to learn more than the submicro structure, but also the electrostatic force – an *interaction*. An understanding of the force is essential for explaining the malleability and ductility of metals. This focus on *interaction* can be considered a progression along different grade levels. It is deemed more valuable than merely describing the structure.

(3) ***Learning* interaction *is more challenging.*** It has been suggested that some students assign 'forces' the properties of 'entities', such as being tangible and consumable, and having weight. Such a designation of forces as entities could make it difficult for students to learn the concept of forces in a scientific way (Chi, 2005). It would be a challenge for students to

learn the electrostatic force (*interaction*) based on their possible knowledge of metals as a *structure*.

While an *interaction* understanding is the highest level of sophistication, a *process* understanding follows as the medium level for the following reasons.

(1) ***Ontological advancement from* structure.** We acknowledge that learning metallic bonding as a *process* is not necessary for an understanding of structure-property relationships. Also, the assumption that metals are formed by metal atoms after each losing their outermost electrons is ungrounded (Taber, 2003a). Nevertheless, a sequential process (*process*) is ontologically different from an entity (*structure)* (Chi, 2013). Acquiring an understanding of *process* is likely to involve a conceptual change that moves away from the *structure* understanding, that is, bonding as 'entities', and thus with the attributes that entities possess. As a *process*, bonding is an idea that is intangible, which is more akin to the *interaction* understanding.

(2) ***As a way to make sense of the new knowledge.*** Although bonding is scientifically an electrostatic attraction rather than a process of forming a product, we argue that having a *process* understanding may serve as a bridge between students' prior learning (e.g., the simple particle model and electron arrangement of atoms), and the new/intended knowledge of the free electron model. Students who have a *process* understanding may assume that individual particles are neutral atoms; metallic bonding forms when these neutral atoms lose the outermost electrons, which become delocalized, and become metal cations. Those who have a *process* understanding may demonstrate an advancement from the simple particle model and an attempt to connect their prior knowledge to the target new knowledge. This may be more desirable than merely recalling *structure*.

(3) ***Lack of property explanation.*** The preceding paragraphs argue that a *process* understanding may be assumed to be more sophisticated than the *structure* understanding.

A *process* understanding, however, fails to consider bonding as an electrostatic force. Thus, among other impediments, a *process* understanding does not help students to explain some of the physical properties of metals at the submicro level. These properties include the strength, relatively high melting and boiling points, and malleability of metals. Therefore, a *process* understanding of metallic bonding is assumed to be less sophisticated than an *interaction* understanding.

This section discusses the assumptions we made in ordering *interaction*, *process* and *structure* at different levels of sophistication. Although *interaction* is considered the most valuable, we did not simply dismissed *process* and *structure* as 'misconceptions' (Smith III, diSessa, & Roschelle, 1993/4). In terms of learning, we would rather see them as potential resources for learning metallic bonding as an *interaction*. In terms of this study, they should more appropriately be considered a synthesis of the literature related to students' understanding of metallic bonding based on Chi's ontological categories of understanding. These categories of understanding thus form the basis of our research question, data collection, and data analysis.

Research Question

Chi's framework has informed the learning of various key scientific concepts. They included electricity, forces (of Newtonian mechanics), and diffusion. Yet, its range of application has been underexplored in chemistry contexts. We envisaged that her framework could also inform how students might understand metallic bonding. Based on the assumptions discussed in the previous section, we hypothesized three increasing levels of understanding; in sequence they were *structure, process* and *interaction*. In this study, we

"tested whether these three categories of understanding metallic bonding were at an increasing level of difficulty".

Students' understanding of metallic bonding has mainly been explored via interviews or small-scale studies (e.g., de Posada, 1997; Taber, 2003b; Coll & Treagust, 2003; Cheng & Gilbert, 2014). These studies have provided much insight into students' understanding. The current study synthesized students' understanding of metallic bonding and tested its hypotheses based on a large sample of students. An answer to the research question would advance our knowledge of how students in general might understand metallic bonding. This study can be likened to some large-scale studies (e.g., Tan et al., 2008; Taber et al., 2012; Johnson & Tymms, 2011) that have tested the findings of earlier qualitative studies. It also contributes to the discussion about how students may advance their thinking about chemistry (e.g., Talanquer, 2009).

Methodology

Sampling

A survey was conducted to answer the research question. All of the secondary schools that adopted the Hong Kong senior secondary level (Years 10-12) chemistry curriculum were invited by e-mail to participate in the study. We requested that all Years 10-12 students taking chemistry at the schools write a short assessment related to their understanding of metallic bonding. Four hundred and fifty e-mails were sent out. Thirty-four schools accepted our invitation.

The Instrument

There were four questions in the instrument (Appendix 1). The design of the instrument was guided by the assumption that the understanding of the free electron model was a hidden trait. Such a hidden trait was measured by the students' views of metallic bonding as an electrostatic force (an *interaction*), a *process* or a *structure* (measured in Questions 1 and 2), their choice of the free electron model to explain the malleability of metals (measured in Question 3), and their ability to explain the malleability based on the *interaction* (measured in Question 4).

In Question 1, the students were asked to choose a figure from six options (Figures 1-6) that best fit their understanding of metallic bonding. The design principles of the options were as follows.

– Figures 5 and 6 were representations of *structure*. The pair of diagrams in Figure 5 showed electrons located at different places. In Figure 6, the electrons were located only outside the metal cations. We created this option based on an observation from previous studies (Cheng & Gilbert, 2014; Coll & Treagust, 2003) that some students considered that the electrons surrounded the whole lattice (a 'wrapping model').

– Figures 1 and 2 were representations of the *process* in which metal atoms transformed into metal cations and delocalized electrons. The structure of the free electron model in Figure 1 was scientific. Similar diagrams could also be found in some official curriculums (e.g., AQA, 2010, 2012). The diagrams in Figure 2 were based on the 'wrapping model', which was alternative to accepted science.

– Figures 3 and 4 were representations of *interaction*. Figure 3 highlighted the all-directional attraction between (i) a single electron and its surrounding metal cations, and (ii) a single metal cation and its surrounding electrons. Figure 4 was based on the 'wrapping model'. Also, the attraction was merely limited to single electrons attracted to single metal cations. They characterized alternative ideas reported in the literature that

in a cluster of oppositely charged particles, such as in an atom (with protons and electrons), in an ionic lattice (with cations and anions), or in two charged spheres (in the context of electrostatics in physics), some students may think that one positively charged particle formed an attraction with only one negatively charged particle (Cheng & Gilbert, 2009; Taber et al., 2012).

Both the visual and verbal means of representations played important roles in learning and assessment (Schnotz, 2005; Akaygun & Jones, 2014; Cooper, Williams, & Underwood, 2015). It was found that students could recall the definition of metallic bonding in words but were unable to draw scientific representations accordingly (Cheng & Gilbert, 2014). Dual coding theory suggested that although the visual and verbal representation systems could work in connection, they could also work independently (Paivio, 2007; Sadoski & Paivio, 2013). Therefore, Question 1 essentially probed into the students' understanding through visual means. Question 2 asked the students to explain their choice in words. Their written explanations revealed their views related to metallic bonding through another means.

Question 3 probed into the students' explanations for malleability and submicro structural changes before/after a piece of metal was pressed. Figures 1 and 5 of this question were based on the simple particle model; the latter was adopted from a commonly reported students' idea that metal atoms were malleable (Ben-Zvi, Eylon, & Silberstein, 1986). Figure 4 was a scientific representation of the free electron model. Figures 2 and 3 reflected the idea that electrons wrapped around the entire metal cation lattice that might protect the metal from falling apart when it was under stress.

Malleability results from the mobility of electrons, which maintain the attraction with metal cations when a piece of metal is pressed. We think it is a limitation of static diagrams that they cannot represent *both* the mobility of electrons and the attraction between the

electrons and cations. We considered using arrows (as in the *interaction* representations in Question 1), but the number of arrows required (between the electrons and cations) would result in the diagram becoming too messy and complicated to be comprehensible. We were unable to find diagrams that represent malleability in terms of electrostatic force (*interactions*), so we used Figure 4 as the best compromise for representing the malleability of metals.

Question 4 asked students to write an explanation of the malleability of metals. This open-ended written question aimed to overcome the limitations of visual representation in Question 3, which did not show electrostatic force as an explanation. We expected that the visual and verbal questions would sufficiently assess the students' explanations for the malleability of metals.

Rasch Modelling

This study aimed to test if *structure*, *process* and *interaction* were at increased levels of understanding. Before we tested this hypothesis, we needed to confirm that the three categories measured only one trait, that is, the understanding of metallic bonding. Psychometrically, this property is called unidimensionality (of different levels). We examined if these three categories are unidimensional by initially running a statistical test on the data. If the statistical analysis revealed they are not, it may mean that the instrument is measuring something else or is poorly set, and if so, identifying if these categories are at different levels would be irrelevant.

We found in our search for an appropriate analysis that the Rasch measurement model meets our research objectives. Rasch modelling allows researchers to determine if an instrument measures a trait that is unidimensional. If the data collected fit well into the Rasch model (the criteria of fit is discussed below), it means that the instrument is

unidimensional. If the data do not fit, the instrument may be measuring different traits other than the understanding of metallic bonding. When the data is found to fit the Rasch model, we can determine the levels of difficulty in *interaction*, *process* and *structure* understanding. To be more specific, we used Rasch's Partial Credit Model (PCM) (Rasch, 1960, 1980) to validate the psychometric properties of the instrument. The statistical software program WINSTEPS (Linacre, 2014) was used for data analyses. The PCM is an extension of Rasch's dichotomous model (Rasch, 1960, 1980) and Andrich's rating scale model (Andrich, 1978). In PCM, scores can be awarded for fully and partially correct answers (Masters, 1982). This matched the requirement of this study, in which an *interaction* was hypothesized as a full understanding, while *process* and *structure* understandings were hypothesized as partially correct answers.

Data Analysis

This section discusses how we conducted the data analysis. First, we report how we coded students' responses in the instrument, then how we examined the psychometric properties of the instrument by Rasch modelling. Last, we report how we determined the levels of difficulty of *structure*, *process* and *interaction* understanding.

Coding of students' answers. Students who chose unscientific diagrams (Figures 2, 4 and 6) in Question 1 received a score of '0' on this question. The *structure* (Figure 5), *process* (Figure 1) and *interaction* (Figure 3) diagrams received scores of '1', '2' and '3', respectively.

Students' written responses in Question 2 were coded in the same way. Unscientific or nil responses received a score of '0'. Responses that (a) mentioned only the *structure* received a score of '1', (b) described the *process* received a score of '2' and (c) referred to the

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attraction or electrostatic force between electrons and metal cations (*interaction*) received a score of '3'. Some quotes from the sample are provided as follows:

"There are free electrons in the metallic bonding, … it was known as the sea electrons. That can move freely around the whole metallic bond." (Score: 1)

"The metals will lose electrons to become metal ions, and the mobile electrons can move freely around the ions." (Score: 2)

"It has an electrostatic force between ions and free electrons." (Score: 3)

Question 3 assessed the students' explanations for metal malleability. Those who chose unscientific diagrams (Figures 2, 3 and 5) received a score of '0' on this item. Those who chose the simple particle and free electron models received scores of '1' and '2', respectively. In Question 4, nil responses received a score of '0'. Written responses such as the following that mentioned only the structural change or structure of the metals received a score of '1':

"free electrons moving in the metals cause the malleability of metals. Due to the sea of electrons, the metals are malleable, it will not be broken easily."

Although this answer mentioned electrons as structural components, it did not make the cause of the property explicit. Thus, it received a score of '1' rather than '2'.

Responses such as the following that explained the property in terms of the electrostatic force or attraction (*interaction*) received a score of '2':

"although you pull the metal, ... because there is electrostatic force between ions and electrons… Therefore it shows that metals are malleable due to metallic bond."

The written responses were coded by the first author and a research assistant with a bachelor degree in chemistry and a doctorate degree in science education (chemistry teachers' pedagogical content knowledge). The research assistant was informed by the first author of the *structure*, *process* and *interaction* understanding of metallic bonding, and was

referred to relevant journal articles before coding. The first author worked with the research assistant in the coding of 36 scripts. They then independently coded 298 scripts obtained from three schools. The percentage agreement of inter-rater reliability of these 596 items was 97.1%. The disagreement was discussed until a consensus was reached. The research assistant then completed the rating of the rest of the scripts.

Rasch analysis – psychometric properties of the instrument. The key parameters for the psychometric properties of the instrument are described below. The discussion includes how we determined the dimensionality of the data, whether the instrument was gender unbiased and whether it fitted well with the student sample.

(a) Model-data fit: This indicates whether the actual data are close to the expectations of the Rasch model (Bond & Fox, 2015). Data within the model-data fit can be interpreted as unidimensional (i.e., meeting Rasch's expectations), that is, the items measured only one latent trait (Bond & Fox, 2015), which is students' understanding of metallic bonding.

The model-data fit is assessed by an 'infit' and 'outfit' mean square (MnSq). An infit and outfit MnSq ranging between 0.50 and 1.50 indicates good adhesion (Thomas, Anderson, & Nashon, 2008; Wright & Linacre, 1996). When the MnSq falls outside the range ('misfitting'), the data do not fit the Rasch model and may measure more than one latent trait. The instrument may be measuring something other than students' understanding of metallic bonding.

(b) Dimensionality: Principal Component Analysis (PCA) of residuals identified a potential secondary dimension ('noises') in the data (Linacre, 2014). It indicates whether the noises are substantial enough to distort the measurement of students' understanding of metallic bonding.

In the survey, if 50% of the 'raw variance' (i.e., observation from raw scores) is explained by Rasch measures, the data can then be assumed to be unidimensional (Linacre, 2014).

(c) Invariance: No previous studies focus on gender differences in understanding metallic bonding. We believe it is important that the instrument works equally across genders. An analysis that indicated 'invariance' across genders could ascertain this. The Differential Item Functioning (DIF) analysis examined whether the instrument functioned differently between sub-samples (e.g., male *versus* female students, different races). A non-significance DIF assumes an invariance property where the instrument functions well with no bias against any particular sub-groups (Bond & Fox, 2007).

Rasch modelling analysis transformed raw scores into 'Rasch measures' (with the unit *logit*) for each item. The Rasch measures for the items are the 'item estimates', which indicate the difficulty of an item. The higher the item estimate, the more difficult the item. In the DIF analysis, each item estimate with respect to male students ('DIF measure for male students') and to female students ('DIF measure for female students') were calculated. The difference between the DIF measures of an item for male and female ('DIF contrast') indicates the difference in item difficulty between the two genders. The difference must be at least 0.50 logit for gender differences to be noticeable and considered significant (Linacre, 2014).

(d) Targeting: Rasch modelling analysis also generates another 'Rasch measure' from raw scores called the 'person estimate'. Each student has a person estimate, which indicates his or her ability in answering the instrument. Rasch analysis allows us to examine if the instrument targeted the sample well. An 'item-person map', which tabulates item estimates and person estimates in a scale (shown in Figure 1 and described in its caption), can indicate whether the difficulty of items matched well with students' understanding

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of metallic bonding (Bond & Fox, 2015). We aimed to avoid situations where the test is too easy or too difficult for the intended students, as this will not reveal their understanding of the concept.

Rasch analysis – levels of difficulty. After the psychometric properties of the instrument were identified, the levels of *structure*, *process* and *interaction* understanding were determined. The previous subsection (c) 'Invariance' discussed the 'item estimate' for each item. Rasch modelling also allowed us to calculate item estimates for *structure*, for *process* and for *interaction* understandings for items 1 and 2, and for *structure* and *interaction* for item 4. That is, an item estimate can be found for each choice within these items. These item estimates reflect the difficulty of *structure*, *process* and *interaction* understanding. If these categories of understanding followed an increasing level of difficulty, the item estimate for *interaction* would be the highest and that for *structure* the lowest.

Findings

This section starts by briefly reporting the pilot results. The psychometric properties of the instrument are then discussed. These include the unidimensionality of the data, the measurement of invariance across genders, and the appropriateness of the items for the samples. Next, results pertaining to the research question, that is, analysis that reveals the increasing difficulty of *structure*, *process* and *interaction* understandings of metallic bonding, are reported.

Pilot

A pilot test was conducted with 549 students at six secondary schools, including 188 Year 10, 190 Year 11 and 171 Year 12 students. The data were subjected to Rasch analysis to examine

the psychometric properties of the instrument. Fit statistics, PCA of residuals and DIF contrast of the two genders were examined. Infit MnSq ranged from 0.65 to 1.17 and outfit MnSq varied from 0.78 to 1.27. All of the items stayed within the acceptable fit range (0.50-1.50). PCA of residuals analysis indicated that about 50% of raw variance was explained by Rasch measures. There was no strong evidence of the presence of a secondary dimension in the data. None of the items reported DIF contrasts of more than 0.50 logit, meaning that the items functioned the same way across the two genders. The pilot results revealed that the instrument could reliably measure what it was intended for.

Main Study

The main study involved 3,006 students, including 1,114 Year 10 students, 1,000 Year 11 and 892 Year 12 students. Of these students, 1,155 were boys and 1,136 girls, while 715 did not indicate their gender. Data were subjected to Rasch analysis to examine the psychometric properties of the instrument and to interpret the students' understandings of metallic bonding.

Part 1: Psychometric properties of the instrument. Table 1 presents item statistics for the four items. It indicates whether they showed acceptable fit with the Rasch model. Based on the aforementioned criteria for the MnSq fit statistics, in general, the data garnered from the test yielded a good fit. All of the items stayed within the acceptable MnSq infit and outfit statistics (0.70-1.29), satisfying the expectation of the Rasch model (in which the acceptable range was 0.50-1.50. All of the items showed moderate to strong correlations (0.61-0.70). This is another piece of evidence indicating that the data were unidimensional (Mok, Cheng, Moore, & Kennedy, 2006). PCA of residuals confirmed this, as 45% of the raw variance was

explained by Rasch measures. Thus, it can be stated confidently that the assumption of unidimensionality held for the data used in the present study.

[Table 1 here]

Table 2 presents the DIF statistics for the male and female students. Although some students did not indicate their gender, 76% (2,291 out of 3,006 students) did. They are representative of the whole sample. None of the items displayed a DIF contrast equal to or larger than 0.50 logit, meaning that the contrasts between genders were not significant. This indicated the invariant structure of the items for the gender sub-samples.

[Table 2 here]

In this study, the item estimates ranged from 8.74 to 10.79 (Table 1; the third column of Figure 1 shows the range) and the person estimates of the whole sample ranged from 6.82 to 13.15 (the second column of Figure 1 shows the range). The mean of person estimates (10.15) was very close to the mean of item estimates (10.00) (Figure 1). The Person-item map also showed that persons and items clustered opposite each other. The results indicated that the instrument used in this study was appropriate for assessing the students' understanding of metallic bonding.

[Figure 1 here]

Figure 1 facilitates visual inspection of the adequacy of the items as intended. Gaps in the distribution indicate the inadequacy of the items in measuring the latent trait (Thomas et al., 2008), that is, students' understanding of metallic bonding. There was a large gap between the easiest item (Q.3) and second easiest item (Q.2).

*Part 2: Rasch analysis – Levels of difficulty (*structure*, *process* and* interaction*).* The item estimates of Question 1 were 10.02 logits for *structure*, 10.33 logits for *process* and 11.64 logits for *interaction* (Table 3). An increasing difficulty pattern from *structure* to *interaction* was

observed, with a difference of 1.62 logits between them. The same increasing trend held true

for Question 2. The item estimates for *structure*, *process* and *interaction* increased from 9.91

logits, to 10.69 logits and 11.48 logits respectively. A difference of 1.57 logits was observed

between *structure* and *interaction*. The Question 4 data were consistent with those of

Questions 1 and 2. The item estimate for an *interaction* understanding (11.78 logits) was

higher than that for a *structure* understanding (10.46 logits).

[Table 3 here]

Question 3 asked about the submicro structural rearrangement of a metal before and

after being hammered and was the least difficult (Figure 1). The item estimates for Question

3 were 9.52 logits for the simple particle model representation and 10.71 logits for the free

electron model representation. The results suggest that the free electron model appeared to

be more challenging than the simple particle model. At such, those who chose the free

electron model to explain malleability therefore demonstrated a better understanding of

metallic bonding than those who chose the simple particle model.

The findings suggest that the *structure* understanding of metallic bonding presented

a lesser challenge to students than the *process* and *interaction* understandings. The gap

between the *structure* and the *interaction* understandings was apparent in all of the cases. In

other words, the data supported our a priori hypothesis that understanding metallic

bonding as a *structure*, a *process*, and an *interaction* was in an increasing level of difficulty.

In summary, data analysis suggests that the instrument was valid in measuring

students' understanding of metallic bonding as a single latent trait. The invariance property

of measurement shows that the items functioned similarly between male and female

students. The items were appropriate for its use, as they well targeted the abilities of

students. In relation to the research question, the data empirically supported the increasing

levels of difficulty of *structure*, *process* and *interaction* understandings of metallic bonding.

Discussion

This large-scale survey was informed by the general framework proposed by Chi (2005; 2013), which indicated that learning an emergent process would pose a big challenge to students. This study also provided a novel example (*viz.* the free electron model of metallic bonding) of an emergent process in which the learning was challenging. This example was different from those proposed by Chi (2005; 2013), which stated that mis-categorization led to unscientific understanding. In our case, an understanding of the free electron model could have related to its *structure*, *process,* or *interaction*. Although the *structure* did not offer explanations for some specific properties of the metals, it still could form a basis for the explanation of, for example, heat and electrical conductivity. Although the *process* could be unnecessary for an understanding of metallic bonding as an electrostatic force, it might serve as a bridge between the simple particle and free electron models.

We hypothesized that these categories were unidimensional and at different levels of sophistication, and presented different levels of difficulty to students. It was found that understanding metallic bonding as an *interaction* (an emergent process), which was the most sophisticated category of understanding, was the most difficult and challenging to students. Understanding metallic bonding as a *process* (a sequential process) was less challenging, and understanding it as a *structure* (an entity) was the least challenging.

We could postulate from the findings that learning the free electron model of metallic bonding is likely to involve a conceptual change when students hold a *structure* understanding. Such an understanding may relate to students' prior learning of the simple particle model in Years 7-9, in which the focus was the structural arrangement of particles. If students apply the same category of understanding in their learning, they may just focus on the electron sea and metal cations of the free electron model. It is likely to be the case when

students regard progressive learning of science as a more detailed or realistic description of natural phenomena (Grosslight, Unger, & Jay, 1991). It may also explain why it was tempting for some of the students to explain the malleability of metals in terms of the structural rearrangement of metal cations. To these students, the structural change at the submicro level might have already provided a sufficient and satisfactory explanation of the property.

The findings also suggest that learning metallic bonding as an *interaction* involves a conceptual change when students hold a *process* understanding. The *process* understanding is consistent with the idea that ionic bonding is a process of electron transfer and covalent bonding is a process of electron sharing (Taber, 2001; 2003a). Although this understanding is not conducive to explaining malleability, the data suggested that having a *process* understanding was more sophisticated than having merely a *structure* understanding. It is likely to be related to Chi's proposition that a process understanding is ontologically different from an entity understanding. Both the sequential process (*process* in this study) and emergent process (*interaction*) share similarities. In this case, for example, bonding is intangible, does not occupy space and does not have mass. It may be less challenging for students to undergo a conceptual change to adopt an *interaction* understanding when they hold a *process* understanding than those who hold a *structure* understanding.

Interview and small-scale studies are beneficial because they allow an in-depth exploration of students' understanding. Insights generated from these studies may be tested in large-scale studies. It has been demonstrated that the results of small-scale investigations of students' learning of, for example, ionization energy (Taber, 1998) and concepts of substances (Johnson, 1998) could be verified in large-scale studies (Tan et al., 2008; Johnson & Tymms, 2011). This study lends support to the validity of small-scale interview studies on

students' learning of metallic bonding (e.g., Cheng & Gilbert, 2014). The quantitative study involving 3,006 Year 10-12 students supported the insights gained.

The study also contributes to the literature of conceptual change. Chi's ontological categories have been useful to researchers attempting to make sense of students' challenges in learning scientific concepts. This study tested her ideas on students' understanding of metallic bonding. Traditional testing can only reveal the percentage of students who choose different categories of understanding. Using Rasch, it was possible to measure the difficulty level of different categories, and this hierarchy of different ontological categories has not been previously investigated. Our findings open new research directions, and raise the question of whether the hierarchy of understanding applies to students' understanding of covalent bonding and ionic bonding.

Conclusion

In this study, we developed a validated instrument that assessed students' description of metallic bonding as an all-directional electrostatic force (i.e., an *interaction*) and their explanations for the malleability of metals based on such an *interaction*. Items were found to possess good psychometric properties: they exhibited moderate to strong correlations (0.61-0.70), targeted the abilities of students well and were not gender biased. We hypothesized that there were different ontological categories of understanding metallic bonding, and that the categories of *structure*, *process*, and *interaction* were at an increasing levels of sophistication and difficulty. The instrument was administered to 3,006 Years 10-12 students who were studying chemistry. The hypothesis was borne out using the Rasch PCM. Many studies have examined students' learning of ionic and covalent bonding. This study addresses knowledge gaps in the literature by identifying patterns of students'

understanding of the structure, bonding and properties of metals (specifically in a context where students have only previously learnt the *structure* of the simple particle model). It also advances Chi's ontological categories of the understanding of scientific concepts in three ways. First, it lends support to her model through a large-scale survey. Second, it offers a novel example of her model, namely, the learning of metallic bonding in school chemistry. Third, this novel example covers a range of understandings of the same scientific concept. They include those related to the emergent process (*interaction*), sequential process (*process*) and entity (*structure*). We acknowledge that an *interaction* understanding is the most desirable. However, a *process* or *structure* understanding cannot simply be dismissed as misconceptions. The focus should be drawn towards ways to support students' learning of the *interaction* based on their possible *process* and *structure* understanding.

Implications for Teaching and Learning

(1) There were two conditions for a conceptual change from one category of understanding to another (Chi, 2013). First, students must be aware that they have made a category mistake. Second, students must be knowledgeable about the correct category (i.e., bonding as an *interaction* in this study).

Some textbooks and official curriculum documents have represented metallic bonding as a *structure* and a sequential *process* respectively (Cheng & Gilbert, 2014; AQA, 2010, 2012). When teachers teach according to the information provided in these textbooks and curriculum documents, it is likely that they are providing their students with information that does not facilitate their understanding of bonding as an *interaction*. We conjecture that some students were not made to be aware of *interaction* being the target of their learning. Therefore, we suggest that a first step towards helping students to learn metallic bonding as an *interaction* is to explicitly teach that the electrostatic force is an

interaction between electrons and metal cations. We believe that it is imperative for textbook authors, curriculum developers, and teachers to abandon representations of bonding merely as a *structure* and/or a sequential *process*. Words and diagrams should consistently represent metallic bonding as an electrostatic force. Diagrams similar to that in Figure 3 of Question 1 may be used for such a purpose. In classroom teaching, the affordances and limitations of a *structure* and *process* understandings in relation to the learning of *interaction* should be discussed with students.

As an emergent process, all agents behave in a more or less uniform way simultaneously (Chi, p.65, Table 3.2). One of the keys to *interaction* is the presence of a reciprocal and simultaneous electrostatic attraction among each electron and each cation in a metal lattice. Such a feature is extremely rare in students' daily experience. Although students could state qualitative relationships in Coulombic electrostatic law and apply such relationships in some submicro structures, they might tend to believe in one-to-one attractions (Lee & Cheng, 2014). Given that some explicit training has been found to be conducive to students' learning of some emergent phenomena (Slotta & Chi, 2006), and that students might readily apply Coulombic electrostatics in some simple situations, we would suggest that the reciprocal and simultaneous interaction between metal cations and electrons at various distances should be discussed explicitly in the teaching of metallic bonding. If students have also learned ionic bonding as an all-directional electrostatic force, it would be worthwhile where appropriate to draw on that possible *interaction* understanding between ions in the learning of metallic bonding. In this way, students' *process* understanding of both ionic and metallic bonding would be challenged.

(2) The findings also have strong implications for the teaching and learning of metal malleability based on the free electron model. We acknowledge that students should be asked to construct models of physical phenomena (Oliveira, Justi, & Mendonça, 2015). In a

similar way, after students are introduced to the free electron model, teachers may ask them to generate an explanation based on the model. Although this strategy is fruitful for students' learning, it is likely to place great demands on the expertise of teachers. We would like to suggest that after macroscopic properties (such as metal malleability) and the free electron model are introduced (as suggested in the previous paragraph), teachers may present the set or a partial set of diagrams used in Question 3 of the instrument to the class (Further suggestions on the design of diagrams in this question are discussed in the next section). Students can then be asked to discuss and argue their choice of a diagram that best represents their understanding. By argumentation, students should not only argue for their choice, but also be asked to critique diagrams they believe are less accurate and less satisfactory in explaining the property (Henderson, MacPherson, Osborne, & Wild, 2015). In this way, students would compare the use of the simple particle and free electron models in explaining metal malleability. In addition, students may be asked to generate their own diagrams or other kinds of representations if they think none of the diagrams fits their ideas. Such a teaching strategy has been shown to be effective in helping students to construct scientific ideas and cultivate scientific practice (e.g., Tytler, Prain, Hubber, & Waldrip, 2013; Ryoo & Linn, 2014).

(3) The results of this study can inform teachers of the different understandings students have of the free electron model, and particularly how they can interpret and react to students' responses in the classroom (e.g., Bell & Cowie, 2001). It must be emphasized that *structure* and *process* understandings should not be regarded as misconceptions that were to be discarded. Rather, it is important that teachers are able to develop students' responses/understanding. Responses that demonstrate a *process* (instead of *interaction*) understanding may indicate to teachers that students have undergone an ontological shift (from *structure*). Teachers may also acknowledge students' achievements or attempt to link

their probable prior knowledge (e.g., of the simple particle model or atomic structure) with the free electron model. Only after this should they point out and challenge the limitations of the *process* understanding, such as the failure to explain the specific properties of metals.

Limitations of this Study and Further Research

There are three limitations in this study that we would like to emphasize. We are expecting that further studies would be conducted to address these limitations.

(1) When students learn the simple particle model it has been suggested that the attraction between particles should be addressed (Johnson, 1998). This study was conducted in a context where Grade 7 students were taught the *structure* of the simple particle model but not the attraction between particles. The results of this study should therefore be interpreted in the context of the sample. A consideration of the context raises an empirical question: if students have been taught the inherent attraction between particles in Grade 7, would such an early exposure to the attraction facilitate their learning of *interaction* in the free electron model? We thus invite researchers to extend our study, particularly if their studies are in contexts where students are taught attractions in the simple particle model. We believe that lessons can be learnt from comparative studies in which students experience different curriculums.

(2) Although the instrument exhibited good psychometric properties, the gap between Questions 2 and 3 presented a limitation (Figure 1). To enhance the sensitivity of the instrument for students with a below-average understanding of metallic bonding, such a gap could be avoided by asking questions that are within this range of difficulty. The validity of the instrument is likely to be enhanced if this is addressed.

Students could be asked to critique a diagram that presents a myriad number of electrons in a metal lattice. This question would address a way in which some students might have interpreted the 'electron sea' (Taber, 2003b). We expect that students' answers would vary. Some may merely focus on commenting on the *structure*, for example, that the lattice has an excessive number of electrons. At a more sophisticated level, the critique may address the instability of the lattice due to the repulsion of excessive electrons. Such an answer would thus reflect an *interaction* understanding. We envisage that noticing the myriad number of electrons may not be too challenging for the majority of students, and that the diagrams in Question 1 might have given some hints about the structure of the metal lattice. Therefore, we envisage that the difficulty of this question should fill the gap between Questions 2 and 3.

(3) We have noted that in the diagrams of Question 3 there was a change in the metal lattice from simple cubic to hexagonal close packed, before and after the metal is hammered. Although the density of the metal cations/particles as represented in the instrument did not change and we suspect such a representation of phase change is unlikely to affect the result, we believe that in order to be scientifically accurate, there should not be any representations of a phase change when the instrument is further used in classrooms or in further research. Close packed representations should consistently represent a part of the lattice before and before the metal is hammered.

Acknowledgements

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Item	Total Score	Total Count	Item Estimate	Model S. E.	Infit MnSq	Outfit MnSq	Point Biserial Correlation
Q.1	3,782	2,969	10.37	0.02	1.21	1.29	0.61
Q.2	4,123	2,868	10.10	0.02	0.89	0.92	0.70
Q.3	4,464	2,957	8.74	0.03	1.19	1.07	0.64
Q.4	2,190	2,821	10.79	0.03	0.70	0.78	0.65

Table 1. Item statistics from Rasch analysis

Item	Gender	DIF Measure	DIF Contrast
Q.1	Male	10.28	-0.33
	Female	10.61	
Q.2	Male	10.16	0.14
	Female	10.02	
Q.3	Male	8.74	0.07
	Female	8.67	
Q.4	Male	10.84	0.20
	Female	10.64	

Table 2. Differential Item Functioning (DIF) statistics for male and female students

Item	Data Code	Item Estimate
Q.1	*Structure*	10.02
	Process	10.33
	Interaction	11.64
Q.2	*Structure*	9.91
	Process	10.69
	Interaction	11.48
Q.3	Simple particle model	9.52
	Free electron model	10.71
Q.4	*Structure*	10.46
	Interaction	11.78

Table 3. Item estimates for different response categories

```
Logit          Sampled student              Item
scale

13                       .###   +
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                                 |
                                 |
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                              T|
                         .###   |
12                              +
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                         .###   |T
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                           .  S|
                         .####   |
11                              +
                                |S          Q4
                     .#######   |
                           .    |
                           .    |            Q1
                 .###########   |
                           .    |
                             M|             Q2
10                       .   +M
                           .    |
                  .#########   |
                                |
                           .    |
                                |
                           .    |
                  .######   |S
9                        .  S+
                                |
                           .    |            Q3
                           .    |
                   .####   |T
                                |
                           .    |
                           .  |
8                        .  T+
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                                |
7                        .#   +
```
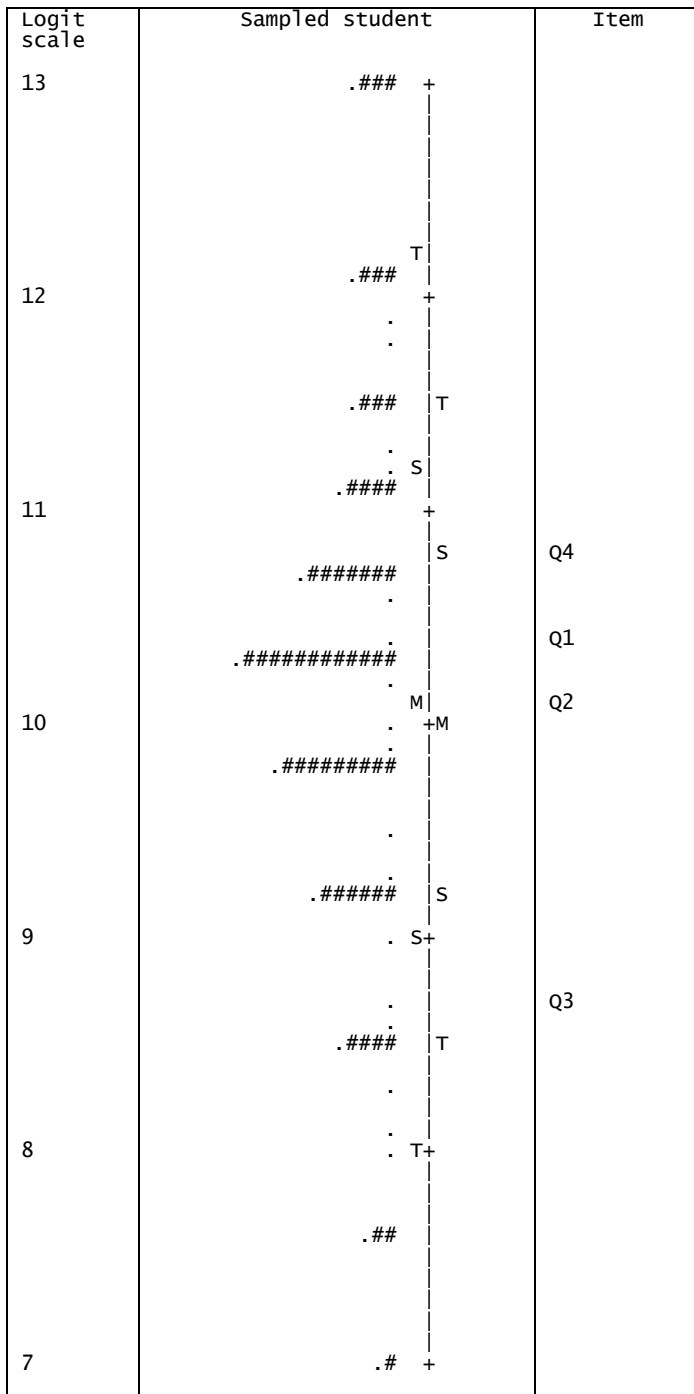
Figure 1. Person-Item Map (The first column is the logit scale for the item and person Rasch measures. The second and third columns are the distributions of students and items, respectively. Each '#' represents 47 students and each '.' represents 1-46 students. The 'M' on the left and right represent the mean for person estimates and the mean for item estimates, respectively. 'S' represents one sample deviation away from the mean, and 'T' represents two sample deviations away from the mean. From the map, it can be seen that most of the students stayed within one sample standard deviation from the mean.)

1. Metallic bonding may be represented as the following diagrams. Which diagram best fits your idea of metallic bonding?

Legend :

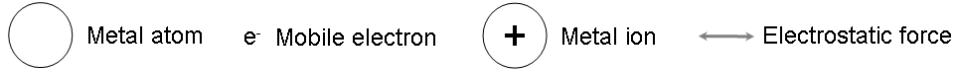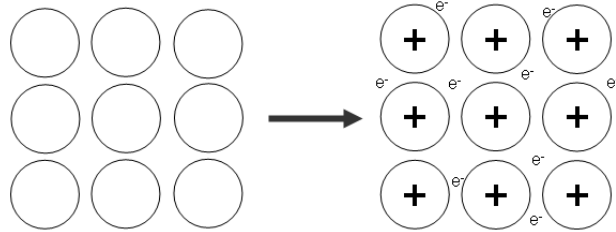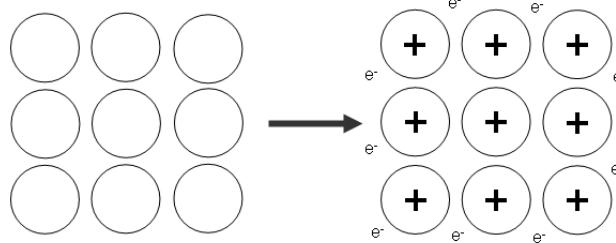◯ Metal atom   e⁻ Mobile electron   (+) Metal ion   ⟷ Electrostatic force
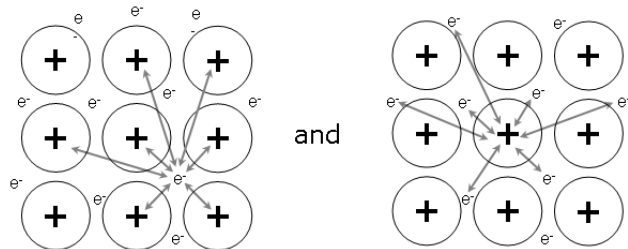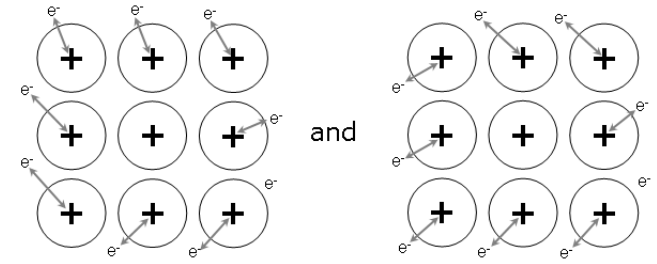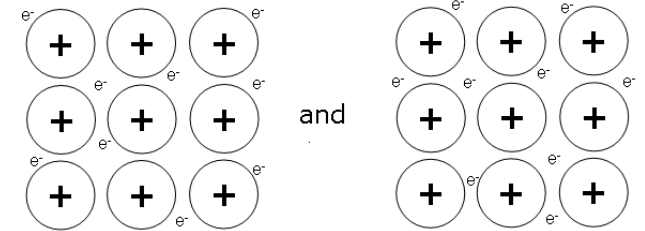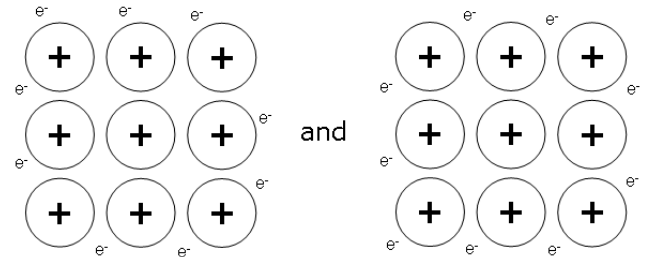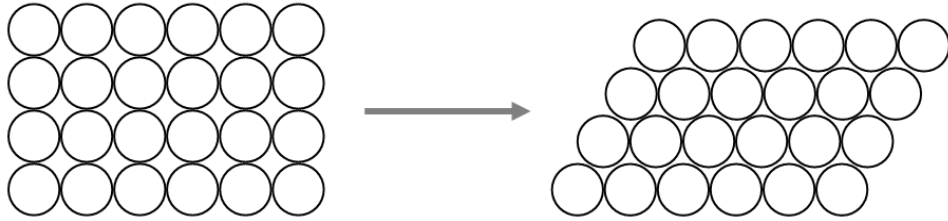
Figure 1

Figure 2

Figure 3

Figure 4

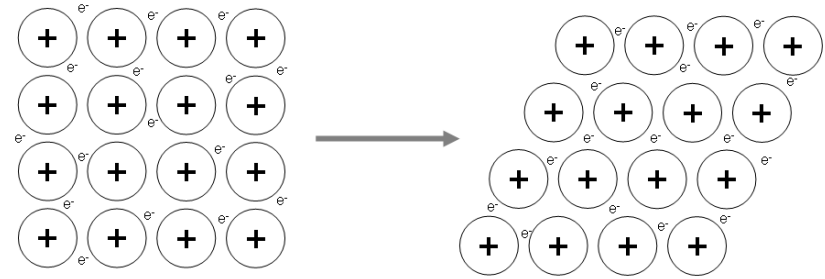Figure 5

Figure 6

Figure ▢ best represents my idea of metallic bonding.

2. It is because _____

_____

_____

_____

_____

3. The malleability of metals may be represented as the following diagrams. Which diagram best fits your idea of the malleability of metals?
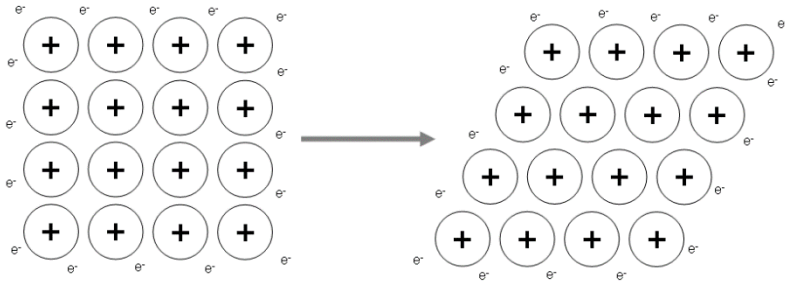
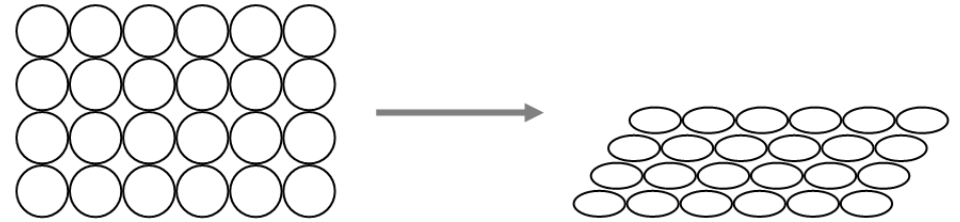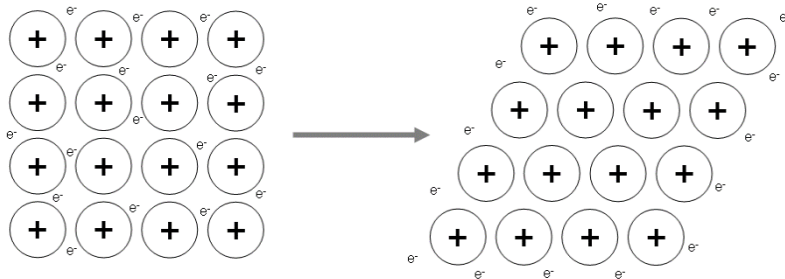**Figure 1**

Figure 2

Figure 3

Figure 4

Figure 5

Figure ☐ best represents my idea of the malleability of metals.

4. In my opinion, metals are malleable because

_____

_____

_____