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Embedded Atom Method Monte Carlo simulation of Cu-Ni bulk alloy

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By

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Table of Contents

Abstract

We have developed a code that implements the embedded atom potentials in conjunction with a Metropolis MC algorithm to investigate some of the thermodynamic properties of the bulk Cu-Ni binary alloy. Calculations were carried out in the semi-grand canonical ensemble—fixed temperature, pressure, number of atoms, and a fixed chemical bias. The results include a plot of equilibrium concentration versus chemical bias, $\Delta\mu$, as well as a plot of a histogram of the probability of finding a specific concentration state. From the latter, we calculated the entropy of mixing, Ω, at 50% copper to be 32.6 $x10^{-3}$ eV/atom which agrees well with a published value of 30 $x10^{-3}$ eV/atom.

Section 1: Introduction

There has been a history of developing numerical simulation methods for the study of different types of alloys. Foiles [1] used the embedded atom method (EAM) in conjunction with Monte Carlo (MC) techniques to study surface segregation phenomena in Ni-Cu alloys. The EAM potential overcame some simulation difficulties associated with using a simple pair-wise body potential. In addition, the computational effort of EAM is only modestly greater than that for a pair-wise potential energy calculation. Foiles also used the Monte Carlo techniques to develop the statistical mechanics of his material. At the time of that work, Monte Carlo methods were fairly well developed and proved successful for varying the composition of a material as well as an atomic scale relaxation of the atoms. Asta and Foiles [2] later used the EAM potential in conjunction with the Monte Carlo technique to study various mean field statistical mechanics properties of a Cu-Ni alloy.

In this work, we develop a code that implements the embedded atom potentials in conjunction with a Metropolis MC algorithm to investigate some of the thermodynamic properties of the bulk Cu-Ni binary alloy. The advantage of this approach is that it is relatively easy to code in comparison with molecular dynamics (MD) techniques, especially working in the semi-grand canonical ensemble. This ensemble places the simulation at fixed temperature, pressure, number of atoms, and a fixed chemical bias. However, we allow the system volume to change, the atoms to move in the crystal lattice, and the number of atoms of each constituent to fluctuate. The fluctuations in constituent concentration contain useful information that we can later exploit.

Section 2: Thermodynamic Theory

Before defining the specific set of variables that will define our thermodynamic states, we need to understand how to utilize Legendre transforms.

A Legendre transform manipulates the variables that are being viewed as independent in a thermodynamic function. In the context of our thermodynamic model, a Legendre transform essentially switches the role of independent variable from one variable to its conjugate variable.

For example, given the Gibbs-Duhem equation for the internal energy in a binary system, where E is the total energy, T is temperature, S is entropy, p is pressure, V is volume, the μ are chemical potentials for atom species 1 and 2, and N_1 and N_2 are the number of atoms of species 1 and 2; respectively.

$$dE = TdS - pdV + \mu_1 dN_1 + \mu_2 dN_2 \tag{2.1}$$

Here E is given as a natural function of S, V, N_1, and N_2.If we needed a natural function of T instead of S, or p instead of V, etc, then we would create a new function via a Legendre transform.

For example, the Helmholtz free energy, A, is given by the Legendre Transform:

$$A = E - TS \tag{2.2}$$

Differentiating here:

$$\begin{aligned} dA &= dE - SdT - TdS \\ dA &= \left(TdS - pdV + \mu_1 dN_1 + \mu_2 dN_2\right) - SdT - TdS \\ dA &= -SdT - pdV + \mu_1 dN_1 + \mu_2 dN_2 \end{aligned} \tag{2.3}$$

Here A is a natural function of T, V, N_1, and N_2. Our goal is to eventually arrive at a natural function of T, p, N, and $\Delta\mu$.

Continuing toward this goal, we define the semi-grand free energy, *Y*, in terms of a Legendre transform of *A*:

$$Y = A - (\mu_1 - \mu_2)N_2 = A - \Delta\mu N_2 \tag{2.4}$$

Similarly:

$$\begin{aligned} dY &= dA - N_2 d\Delta\mu - \Delta\mu dN_2 \\ dY &= (-SdT - pdV + \mu_1 dN_1 + \mu_2 dN_2) - N_2 d\Delta\mu \\ &\quad - \Delta\mu dN_2 \\ dY &= (-SdT - pdV) + (\mu_2 - \Delta\mu)dN_2 + \mu_1 dN_1 - N_2 d\Delta\mu \\ dY &= (-SdT - pdV) + \mu_1 dN_2 + \mu_1 dN_1 - N_2 d\Delta\mu \\ dY &= (-SdT - pdV) + \mu_1 dN - N_2 d\Delta\mu \end{aligned} \tag{2.5}$$

Finally define *W* with the following Legendre Transform:

$$W = Y + pV \tag{2.6}$$

This yields:

$$\begin{aligned} dW &= dY + Vdp + pdV \\ dW &= (-SdT - pdV + \mu_1 dN - N_2 d\Delta\mu) + Vdp + pdV \\ dW &= -SdT + Vdp + \mu_1 dN - N_2 d\Delta\mu \end{aligned} \tag{2.7}$$

This leaves *W* as a natural function of our desired variables: *T*, *p*, *N*, and $\Delta\mu$.

Now define *G*, the Gibbs free energy, as:

$$\begin{aligned} G &= A + pV = E - TS + pV \\ G &= \mu_1 N_1 + \mu_2 N_2 \end{aligned} \tag{2.8}$$

Let $N = N_1 + N_2$ and $C = N_2/N$, resulting in:

$$G = N[(1 - C)\mu_1 + C\mu_2] \tag{2.9}$$

Considering this definition of *G* in conjunction of our definition of *W*:

$$W = N[(1 - C)\mu_1 + C\mu_2 - C\Delta\mu] \tag{2.10}$$

Under conditions of constant temperature *T*, pressure *p*, and number of atoms *N*, *W* is a minimum at thermodynamic equilibrium. For a perfect mixture, we have [3]:

$$\mu_k(p,T) = u_{ko}(p,T) + N_k k_B T ln\left(\frac{N_k}{N}\right), \tag{2.11}$$

In our case we have k = 1,2. Taking this and substituting into the equation for W:

$$W = N[\mu_{10} + \Delta\mu_0 C + k_B T(1-C)\ln(1-C) + k_B T C ln C - C\Delta\mu] \tag{2.12}$$

where $\Delta\mu_0 = \mu_{20} - \mu_{10}$. The log terms in equation 2.12 can be associated with the entropy of mixing.

This idea solution model assumes no interaction between the two constituent elements. The regular solution model introduces a correction term that accounts, approximately, for such interactions. This term can be associated with the enthalpy of mixing.[3] Accounting for this in our equation for W results in:

$$W = N[\mu_{10} + \Delta\mu_0 C + k_B T(1-C)\ln(1-C) + k_B T C ln C + \Omega C(1-C) - C\Delta\mu] \tag{2.13}$$

where Ω is the enthalpy of mixing. A final contribution to the entropy arises from the vibration of the atoms in the system. From Fultz [4], this leads to:

$$W = N[\mu_{10} + \Delta\mu_0 C + k_B T(1-C)\ln(1-C) + k_B T C ln C + \Omega C(1-C) - C\Delta\mu + k_B T ln\left(\frac{k_B T}{\hbar\omega_{11}}\right) + 2k_B T C ln\left(\frac{\omega_{11}}{\omega_{22}}\right) + k_B T C^2 \ln\left(\frac{\omega_{12}^2}{\omega_{11}\omega_{22}}\right)] \tag{2.14}$$

where ω_{11} is the atomic vibrational frequency of a pure crystal of type "1", likewise for ω_{22}, and ω_{12} is the frequency for an equal mixture of "1" and "2".

Now consider an expansion of W about the equilibrium concentration C_{eq}, taking $\delta C = C - C_{eq}$. Note that C_{eq} can be calculated from histogram data for a given value of $\Delta\mu$.

$$W - W_{eq} = \Delta W = \frac{\delta W}{\delta C}\Big|_{eq}\delta C + \frac{1}{2}\frac{\delta^2 W}{\delta C^2}\Big|_{eq}\delta C^2 + \ \ldots \tag{2.15}$$

The requirement that W_{eq} be an equilibrium state implies that W_{eq} has a minimum at $C=C_{eq}$, and hence that:

$$\begin{aligned}\frac{1}{N}\frac{\delta W}{\delta C}|_{eq} = \ & \Delta\mu_0 + \Omega(1-2C_{eq}) \\ & + k_BT\left(lnC_{eq} - \ln(1-C_{eq})\right) - \Delta\mu \\ & + 2k_BTln\left(\frac{\omega_{11}}{\omega_{22}}\right) + 2k_BTCln\left(\frac{\omega_{12}^2}{\omega_{11}\omega_{22}}\right) = 0\end{aligned} \tag{2.16}$$

This is because W achieves a minimum at the C_{eq} value. Furthermore,

$$\begin{aligned}\frac{\delta^2 G}{\delta C^2}|_{eq} &= -2N\Omega \\ &+ Nk_BT\left(\frac{1}{C_{eq}} - \frac{1}{1-C_{eq}}\right) \\ &= -2N\Omega + \frac{Nk_BT}{C_{eq}(1-C_{eq})} + 2k_BTln\left(\frac{\omega_{12}^2}{\omega_{11}\omega_{22}}\right)\end{aligned} \tag{2.17}$$

Now use the fact that the fluctuation quantity ΔW should be Boltzman distributed. Using equation 2.16, this gives

$$f_C(\delta C) \sim e^{-\frac{\Delta W(\delta c)}{k_BT}}, \tag{2.18}$$

and from equation 2.15, neglecting terms higher than the quadratic,

$$\begin{aligned}f_C(c) \sim \exp[\frac{1}{2k_BT}(&-2N\Omega + \frac{Nk_BT}{C_{eq}(1-C_{eq})} \\ &+ 2k_BTln\left(\frac{\omega_{12}^2}{\omega_{11}\omega_{22}}\right)\delta C^2]\end{aligned} \tag{2.19}$$

This has the form of a zero-mean Gaussian distribution, with a known normalizing constant. If the standard deviation, σ, can be calculated from histogram data, then we have:

$$\sigma^2 = \left(-\frac{2N\Omega}{k_BT} + \frac{N}{C_{eq}(1-C_{eq})} + 2\ln\left(\frac{\omega_{12}^2}{\omega_{11}\omega_{22}}\right)\right)^{-1}. \tag{2.20}$$

With this equation we can immediately determine Ω, and then $\Delta\mu_0$ can be found via equation 2.16.

Section 3: Numerical Implementation

Monte Carlo simulation and the Metropolis Algorithm

> "A definition of a Monte Carlo method would be one that involves deliberate use of random numbers in a calculation that has the structure of a stochastic process. By stochastic process we mean a sequence of states whose evolution is determined by random events."[5]

This basic definition from Kalos and Whitlock [5] is a good starting point for a discussion of how we begin to simulate the interaction of atoms in a copper nickel alloy. Consider this idea in conjunction with a general definition of the Metropolis Algorithm. Wikipedia [6] defines the Metropolis-Hastings algorithm as "a method for obtaining a sequence of random samples from a probability distribution." Essentially, our goal is to create an equilibrium state in the alloy and attempt to gather information via random walks about that state. If we assume that there is a single equilibrium, random walks from that equilibrium will explore the probability distribution of states occurring close to that equilibrium.

For our purposes, "equilibrium state" is defined as the lowest energy state available to the alloy. Supposing that any random walk eventually allows us to find the equilibrium state as opposed to a local energy minimum, we define our basic algorithm for a single component system as the following:

Given a state A_o propose a new state A_f, where A_f is an alteration of A_o. We accept A_f as our current state with probability:

$$P = e^{-\frac{\Delta E}{k_B T}} \tag{5.1}$$

Here k_B is the Boltzmann constant, and T is the temperature of the simulation. If P is greater than 1, i.e., $\Delta E<0$, if we accept A_f as our new A_o. In this equation, ΔE is dependent on the difference in energy between the two states. If P is greater than 1, this implies that we have reached a lower energy state than the current one. From a true equilibrium state, all values of ΔE are greater than zero. This acceptance criteria biases us to a lower energy state while allowing randomly walk to higher energy states, this helps to avoid us from falling into a local minimum indefinitely. Moreover, the distribution of energies will converge to the Boltzmann distribution predicted by statistical mechanics.

EAM potential and its Implementation for a binary alloy

The embedded atom model is a method of calculating the internal energy of a solid using two different interatomic potential schemes: a two-body potential, and an N-body "embedding function". The two body potential component is an energy associated between two atoms *i* and *j* in the system under observation. This energy is calculated as:

$$E_2^{ij} = C * \frac{Z\left(R_{ij}\right)^2}{R_{ij}} \tag{5.2}$$

where C is a conversion factor, R_{ij} is the distance between the ith and jth atoms, and Z is a given function of R_{ij}. For a binary alloy, the function Z changes depending on the chemical identity of the two atoms are under consideration. For a Cu-Cu bond, $Z=Z_{Cu}$, while $Z=Z_{Ni}$ for a Ni-Ni bond. For a Cu-Ni bond, the Z function is obtained by taking a geometric average of the other two Z functions, or:

$$Z_{Cu-Ni} = \sqrt{Z_{Cu} Z_{Ni}} \tag{5.3}$$

These functions were taken from the Interatomic Potential Repository Project. [5] These potentials were specifically used in Foiles's work. [7]

The N body energy calculation is a composite function that was similarly taken from the Interatomic Potential Repository Project. The N-body energy function, or the embedding function, is the energy required to place an atom in its current location. In practice, it is obtained from a look-up table. It assumes that the atom is working as an interstitial against the existing electron density. The following equations are used:

$$E_N^i = F(\rho^i) \tag{5.4}$$

where

$$\rho^i = \sum_{i \neq j, j=1}^{N_a} f(R_{ij}) \tag{5.5}$$

Here N_a is the number of atoms in our system. For a binary alloy, let F_A be the embedding function for component *A* and F_B the embedding function for component *B*. Similarly define f_A and f_B as functions for *f* in (3.5) for constituent elements A and B. Now define $\delta_A{}^{\alpha}$ so that $\delta_A{}^{i} = 1$ when *i* is of type A and $\delta_A{}^{i} = 0$ otherwise. Define $\delta_B{}^{i}$ similarly concerning type B. Then for a binary system we have:

$$E_N^i = F_A(\rho^i)\delta_A^i + F_B(\rho^i)\delta_B^i \tag{3.6}$$

where

$$\rho^i = \sum_{i \neq j, j=1}^{N_a} f_A(R_{ij})\delta_A^j + f_B(R_{ij})\delta_B^j \tag{3.7}$$

This adapts potentials for a single constituent model to our binary constituent model. The total energy of the system is the summation of all these individual atom contributions, or:

$$E = \frac{1}{2}\sum_{i \neq j} E_2^{ij} + \sum_{i=1}^{Na} E_N^i \qquad (3.8)$$

Since atoms have weak interactions past a certain interatomic spacing, we can efficiently compute the energy by looking at interactions within a certain "cutoff radius" of the *i*th atom. For Ni-Ni and Cu-Ni interactions, 4.8 angstroms was used as the cutoff radius. For Cu-Cu, 4.95 angstroms was used.

Now that we have the ability to calculate the energy for the binary alloy, we only need to define how to generate a new state A_f before we can use the Monte Carlo algorithm that we defined earlier.

Generation of System States and Details of the Code

For a binary alloy, there are three types of attempts to produce a new state. The first of these changes is simply a perturbation the atom spacing by a small amount in *x, y, and z*. We attempt to set a maximum perturbation value in any one direction such that perturbations are accepted roughly 50% of the time. The value we used for this was determined to be approximately 2% of the copper lattice parameter. The perturbation distances were created via a random number generator as a fractional value of the maximum perturbation value. For this type of change, ΔE in the acceptance criteria (3.1) is defined as:

$$\Delta E = E_f - E_o \qquad (3.9)$$

where E_f is the energy of the new state, and E_o is the energy of the original state.

The second of these changes is a chemical identity switch. Essentially we randomly choose an atom and change it from a Cu atom to a Ni atom or vice versa. For this type of change, ΔE is defined as:

$$\Delta E = E_f - E_o - 1.5k_B T ln(F) - \Delta\mu \tag{3.10}$$

Δμ is a chemical potential bias that is set for each trial run. F is the fugacity ratio, and is dependent on whether the atom was switched from a Cu to a Ni or Ni to a Cu. If an atom was switched from Cu to Ni:

$$F = \frac{58.693}{63.546} \tag{3.11}$$

Similarly if an atom was changed from Ni to Cu:

$$F = \frac{63.546}{58.693} \tag{3.12}$$

Note that in the perfect gas approximation used here, these are just the ratios of the atomic weights of nickel and copper.

The third type of change is a volumetric change. We randomly resize the lattice spacing so as to approximately maintain zero pressure for our simulation. For this type of change, ΔE is defined as:

$$\Delta E = E_f - E_o - 3N_a k_B T ln\left(\frac{G_m}{G_{m_0}}\right) \tag{3.13}$$

Here G_m is the new lattice length, and G_{mo} is the old lattice length.

For our simulations, we set up 2048 atoms in an FCC structure. Typically the simulation is initialized with 1024 copper atoms and 1024 nickel atoms randomly distributed throughout the atomic structure. Periodic boundary conditions are set. An initial calculation of the system energy is done. Then a typical simulation runs

approximately 50,000 Monte Carlo steps. A Monte Carlo step consists of 2048 attempted atomic position perturbations, 10 attempted atom identity switches, and 1 attempted volume change, in that order. Atoms associated with a change are randomly selected, and atoms may be selected more than once in a single Monte Carlo step.

Section 4: Results

For each trial we set several parameters prior to running the code. These parameters were the simulation temperature T, the chemical potential bias $\Delta\mu$, and the number of Monte Carlo steps. From the code we output percent copper concentration, lattice parameter, and total energy of the system. Figure 1 is a typical output of the code, showing the variation in Cu concentration as the Monte Carlo simulation progressed.

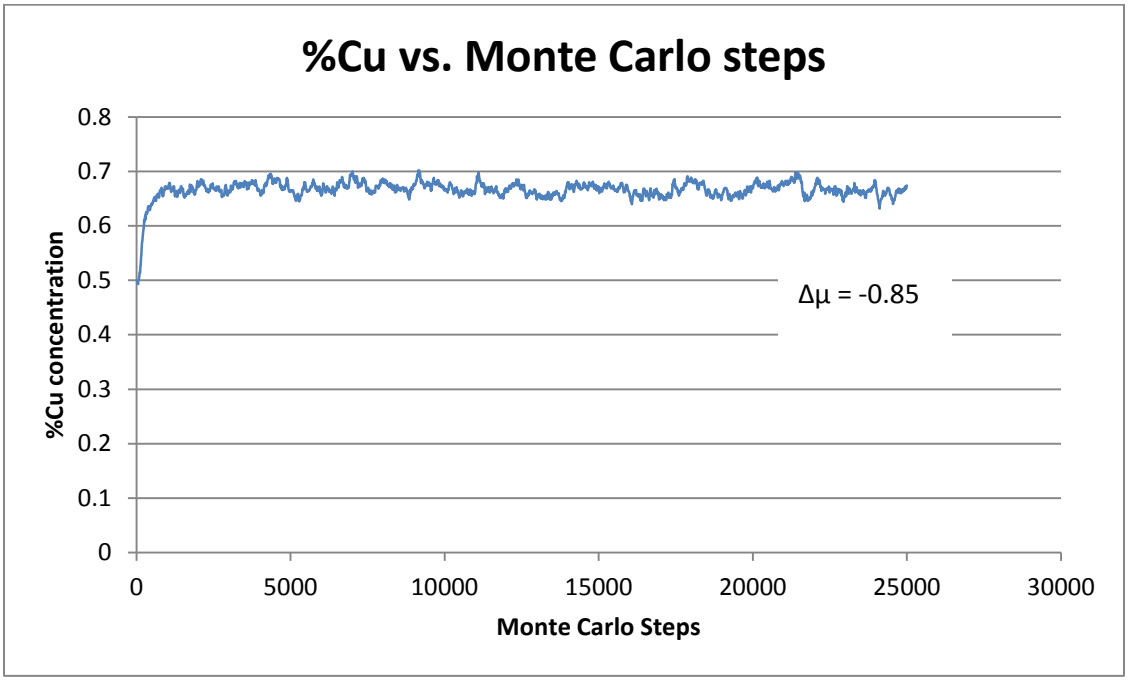

Fig. 1: An example of a simulation output.

In general, we initialized our code at 50% copper –50% nickel. For the trial in figure 1, the temperature was 1100 K, the $\Delta\mu$ value was -0.85, and the number of Monte Carlo steps was 25000. The trial started at 50% copper and moved to equilibrium around 68% copper. Sample points were taken every 10 Monte Carlo steps for this trial. The equilibrium concentration is calculated by determining approximately when the simulation reaches equilibrium and then averaging all data after that point. Here, for

example, this point appears to occur at around 5000 Monte Carlo steps. Note, however, that the concentration fluctuates about the equilibrium value on each Monte Carlo step.

We then varied temperature and $\Delta\mu$ and determined the equilibrium concentrations for those simulations. This result is shown in figure 2. Note here that the 900 K trial has less sigmoidal character than the 1100 K trial. Specifically note the sudden change in slope at $\Delta\mu$=-0.8 in the 900 K trial. This deviation from an odd symmetry about the 50% composition is an interesting phenomenon. In debugging trials of the code at 700 K, strange results were noted around compositions of 50%. In particular, the code couldn't converge to a non-zero percent equilibrium below 50% at 700 K. This is a limitation of this simulation technique. This strange behavior is still somewhat apparent at 900 K.

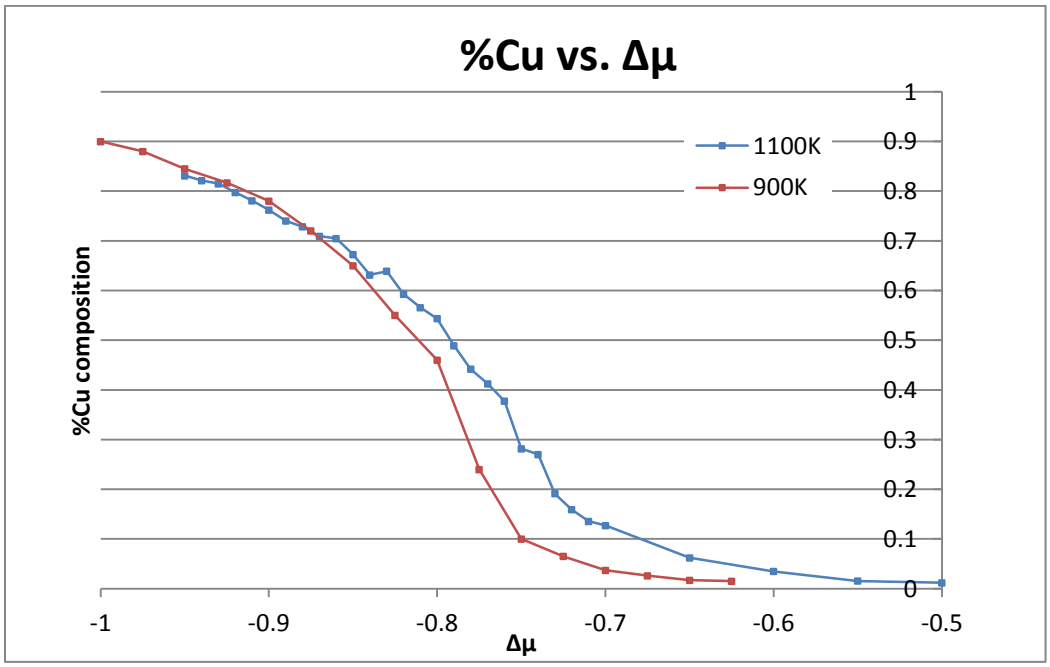

Fig. 2: A plot of %Cu vs. $\Delta\mu$ for 900K and 1100K.

We can also explore the fluctuations in concentration from the equilibrium concentration. An example of this can be found in figure 3, where we plot the value of

the percentage deviation in Cu concentration vs. probability at a specific temperature and $\Delta\mu$.

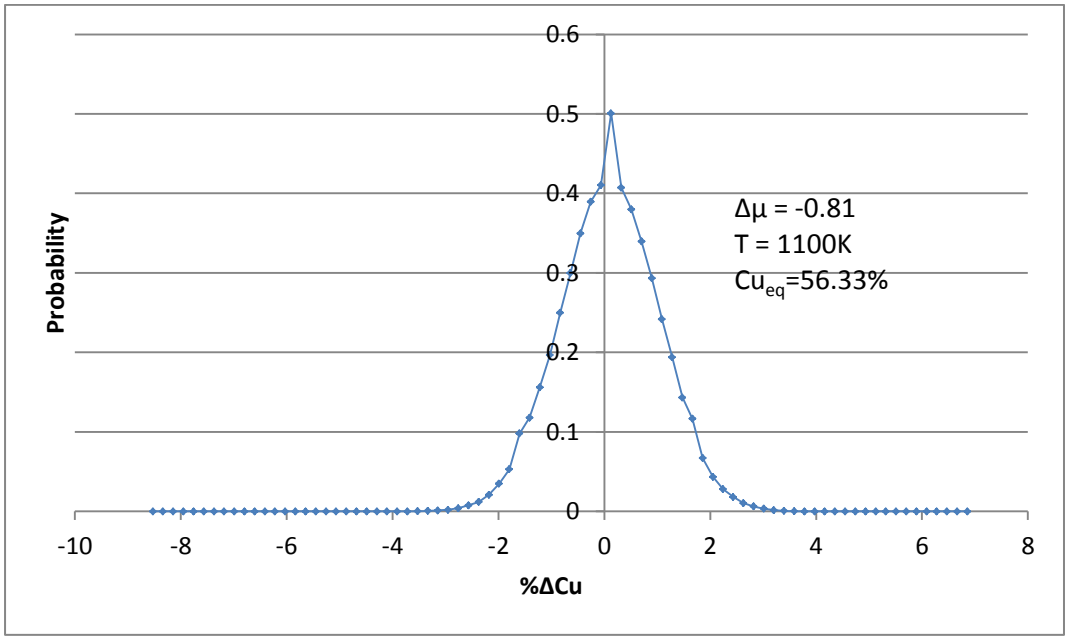

Fig. 3: Probability of finding a %Cu about the equilibrium.

Note that the distribution is qualitatively similarly to a Gaussian distribution, as predicted by equations (2.18-2.19). From the probability distribution, we can calculate the standard deviation and utilize it with equation (2.20). Figure 3 was generated by taking data similar to the data displayed in figure 1 and binning the sample points. The bins used were of size 0.0025. After binning, the bin totals were divided by the total number of samples and the bin size to make the area under the curve unity.

The values of the vibrational frequency, ω, were calculated by taking an atom, in a strictly copper or nickel lattice, and perturbing it a distance Δx then calculating the resulting change in energy. Then we can fit a spring model equation for energy to the data and derive the vibrational frequency from the resulting stiffness k and known atom

mass *m*. Here we have used the fact that for small deviations from equilibrium, the change in energy will be approximately quadratic in the perturbation distance.

$$E = \frac{1}{2}kx^2 \tag{9.1}$$

For nickel we have these results in figure 4.

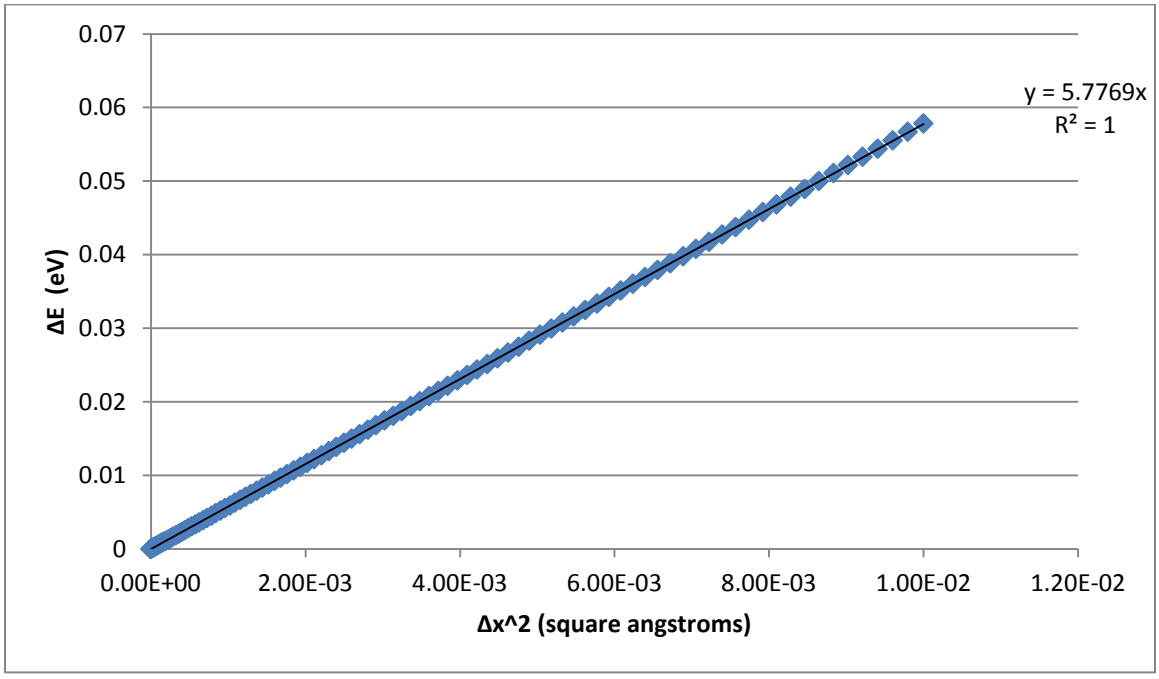

Fig 4. Nickel fundamental frequency trial results. The slope of this line is k/2.

After finding this value of k_{Ni} here to be 11.55 eV/A_o^2, we can use the frequency formulation:

$$\omega = \left(\frac{k}{m}\right)^{\frac{1}{2}} \tag{9.2}$$

Properly accounting for units eventually leaves us with a value of ω_{Ni} = 4.36x10^{13} Hz. Similar calculations were done for copper resulting in a k_{Cu} = 7.01 eV/A^2, and ω_{Cu} =3.26x10^{13}Hz. For our purposes, ω_{11} and ω_{22} refer to these fundamental frequencies of nickel and copper respectively. Moving from (2.20) we use the approximation [2]:

$$\omega_{12} = 0.77(\omega_{11}\omega_{22})^{0.5} \tag{9.3}$$

where this binary fundamental frequency was calculated to be 3.77×10^{13} Hz.

From equation (2.20), taking $C = 0.5$ and using a calculated value of $\sigma^2 = 1.75 \times 10^{-4}$ for a system of $N = 2048$, this gives:

$$\Omega = \frac{k_B T}{2}\left(-\frac{1}{N\sigma^2} + 3.477\right) = 32.6x10^{-3} eV/atom \tag{9.4}$$

This agrees well with a published value of 30×10^{-3} eV/atom in Asta and Foiles [7].

From (2.16) we can calculate $\Delta\mu_0$ from these values. Assuming a $\Delta\mu$ value of -0.79, and having the second and third terms drop from (2.16):

$$\Delta\mu_0 - \Delta\mu + 2k_B T ln\left(\frac{\omega_{11}}{\omega_{22}}\right) + 2k_B TCln\left(\frac{\omega_{12}^2}{\omega_{11}\omega_{22}}\right) = 0 \tag{9.5}$$

$$\Delta\mu_0 = -.79 + \left(8.617 * 10^{-5} * 1100\right)\left(2 * \ln\left(\frac{4.36}{3.26}\right) + \ln(.77^2)\right) \tag{9.6}$$

This results in a $\Delta\mu_0$ value of -0.784 eV.

In the future, there is the possibility of working on reweighting the histograms to extrapolate to nearby points in the thermodynamic parameter space. [8] Similarly, taking the histograms and using cumulant expansion techniques to explore this space is also viable. [9]

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