

Calculation of the Equilibrium Lattice Constants and Stable Lattice Structure of Nickel

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A first-principle study of the various structures of Nickel was conducted in this study. With the quest to determine the most stable structure of the Nickel element, four of the most basic structures including the simple cubic (SC), face-centered cubic (FCC), body-centered cubic (BCC), and the hexagonal close packed (HCP) structure were studied. Based on the gathered data, it was found out that the most stable structure of Nickel is the HCP structure as this structure gave the lowest total energy compared to the other structures. Furthermore, the cohesive energy of this structure was calculated to be zero.

1. Introduction

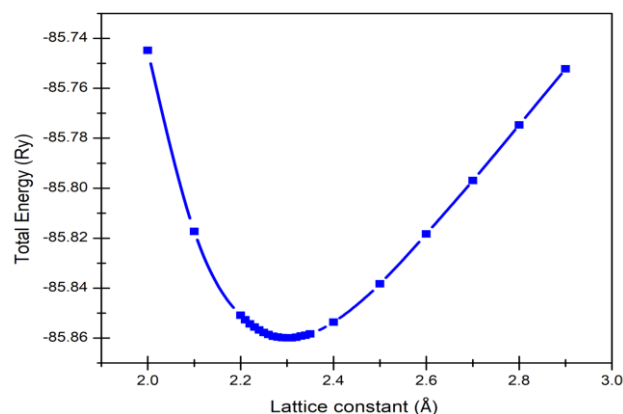
The crystal structures of a material are defined by its lattice constants. While these lattice constants are the most common properties of a crystal system, they play an important role in the electronic properties of the material. Understanding the relations of the lattice parameters and the electronic properties of a system is an important key step in studying the performance of the system in a given condition. Furthermore, gaining enough knowledge on the various microstructure properties of a material are very essential in enhancement or development of the material for certain specific applications.

In determining the most stable structure and consequently the equilibrium lattice constants of a material, one can start looking into the total energy of the system. In general, the total energy of a structure is parabolic as a function of the lattice constant. This parabolic curve has a single minimum total energy. The structure with the least possible total energy is the most stable structure of that certain material. The corresponding lattice constants of this most stable system are automatically the equilibrium lattice parameters of the material. A more meaningful approach however, is by solving the formation energy or the cohesive energy of the system. By definition, the cohesive energy is the amount of energy that is evolved when bringing infinitely separated atoms to form a crystalline solid. This is equivalent to the binding energy of a crystal structure. Hence, the cohesive energy of the most stable structure is zero.

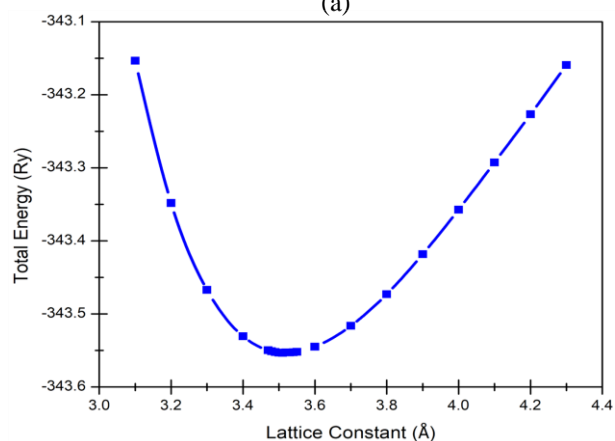
Here, the total energies of the different Nickel structures were computed by applying the Density Functional Theory (DFT). The DFT calculations were done using Quantum Espresso. Among the considered structures are the simple cubic (SC), the face-centered cubic (FCC), the body-centered cubic (BCC), and the hexagonal close packed (HCP).

2. Results and Discussion

For each of the mentioned structures, the total energy was computed at different values of lattice constants. In the SC, FCC and BCC structures, the lattice constant a was varied at satisfactory increments in order to determine the lowest possible energy of each structure. In Figure 1, the



(a)



(b)

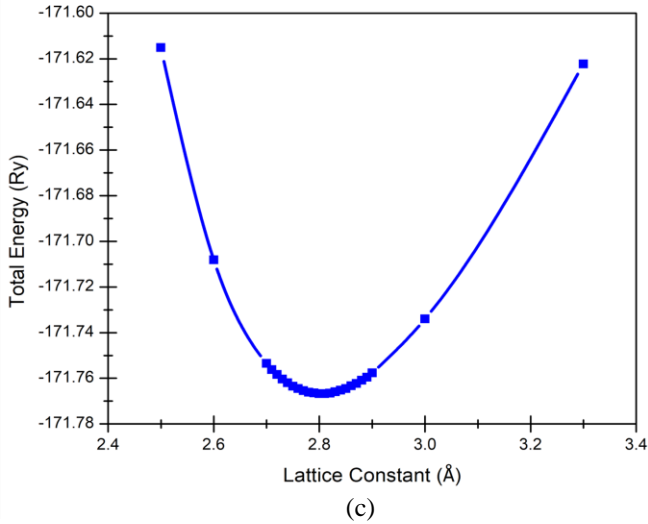


Figure 1: These plots shows the total energy in Rydberg at different values of lattice constants a in Angstrom (Å) for the (a) SC, (b) FCC and (c) BCC structures

total energies in Rydberg (Ry) of each structure are plotted with respect to the lattice constant a in Angstrom (Å).

For the HCP structure, the total energy was calculated at different values of lattice constant a for a number of crystallographic c/a ratio around the ideal value of 1.63. The results for this are shown in Figure 2 below.

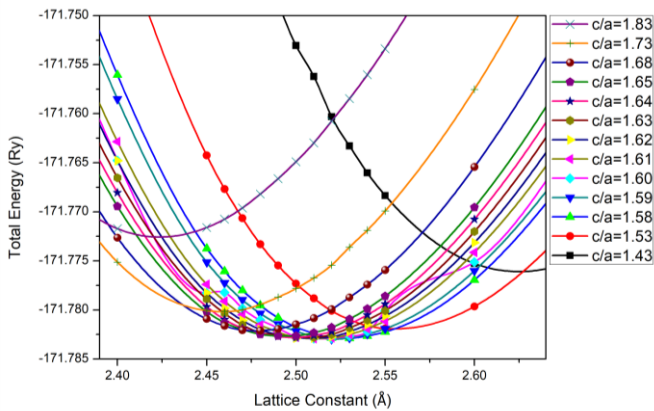


Figure 2: These plots shows the total energy of the HCP structure with respect to the lattice constant a for differenet values of crystallographic c/a ratio about the ideal value of 1.63

Among the results plotted in Figure 2, the minimum energy for the HCP system belongs to the curve for ratio value of $c/a = 1.59$. This curve is shown in Figure 3.

As observed on the presented data, all of the results shown in Figure 1, 2 and 3 portray parabolic curves about a single minimum value of the total energy. The corresponding lattice constants at these minimum energies are the equilibrium lattice constants of each respective

structures. Here, it was found out that the equilibrium lattice constants for SC, FCC, BCC, and HCP are 2.30 Å, 3.51 Å, 2.80 Å, and 2.52 Å, respectively. Furthermore, the equilibrium lattice constant ratio for the HCP structure

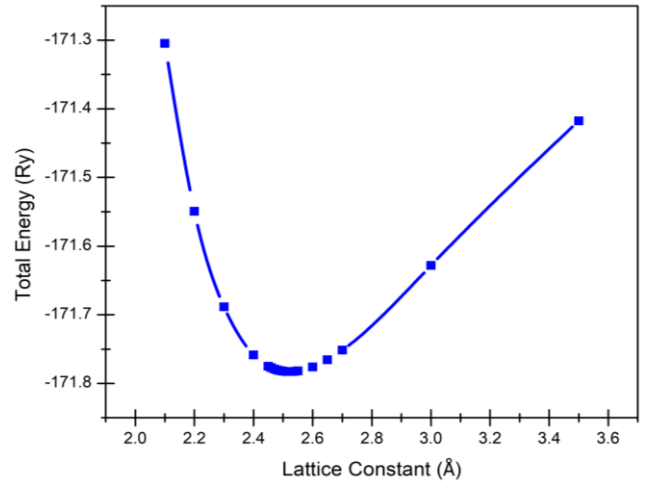


Figure 3: This plot shows the total energy in Rydberg at different values of lattice constants a in Angstrom (Å) for the HCP structure with $c/a = 1.59$

was determined to be $c/a = 1.59$ which is about 2.45% lesser than the ideal value.

The calculated minimum energies were then divided by the number of atoms for each corresponding structure to obtain the chemical potential μ (free energy per atom) for each structure. Then the minimum value μ_{min} of all the calculated chemical potentials was used to solve for the cohesive energy E_{coh} using the following equation:

$$E_{coh} = E_{tot} - n\mu_{min}$$

where E_{tot} is the total energy of the system, n is the number of atoms in a unit cell, and μ_{min} is the chemical potential. The summary of the calculated data is shown in Table 1 below:

Table 1. Calculated chemical potential and cohesive energy

Structure	No. of atoms per unit cell	Lattice constant (a)	Minimum Total Energy	Chemical Potential (μ)	Cohesive Energy
SC	1	2.30	-85.8599233	-85.8599233	0.031566015
FCC	4	3.51	-343.5534238	-85.88835596	0.01253342
BCC	2	2.80	-171.7667171	-85.88335856	0.01626152
HCP	2	2.52	-171.7829786	-85.89148932	0

The highlighted figure in Table 1 is the minimum value among the calculated chemical potentials. Hence, the results suggest that the most stable structure of the Nickel metal is the HCP structure. For better comparison among the values of the cohesive energies of each structure, please refer to Figure 4.

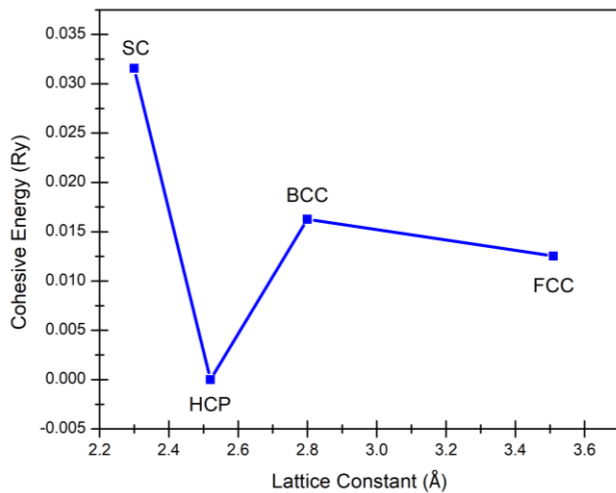


Figure 4. This plot shows the cohesive energy for each considered Ni system.

The obtained cohesive energy value for the HCP structure is zero since based on the presented data, it is the most stable structure of Nickel. This is unfortunately, in contrast to the results presented in the previous studies [1, 2] showing that the most stable structure for Nickel is the FCC structure. This difference in the results may be due to the metastability of the HCP structure. The metastability of HCP Ni predicted was predicted in [1] while it was qualitatively shown in [3] that a slight variation in the c/a ratio from the ideal value would stabilize the HCP structure in either the HCP or the FCC stability range. On the bright side, the equilibrium lattice constant of the FCC nickel coincides with the DFT calculations on the ground state properties of FCC Nickel by [4] and the experimental value in [5].

3. Conclusion

With the DFT calculations, the total energies of Nickel in the SC, FCC, BCC, and HCP structures were determined. Using the lowest total energy, the equilibrium lattice constants of this metal were found out to be $a=2.52$ Å and $c/a=1.59$ Å which corresponds to the HCP structure. Furthermore, the chemical potential and the cohesive energy for each system were also computed.

Based on the gathered data, it can be concluded that the most stable structure of Nickel is the HCP structure.

Computational Model

DFT calculations was implemented using Quantum Espresso with exchange-correlation term described using the generalized gradient approximation (GGA) based on Perdew-Burke-Ernzerhof (PBE) functional. The interaction between ions and electrons was described using the projector augmented wave (PAW) method.

Plane wave basis sets was employed with an energy cut-off of 250 Ry. The surface Brillouin zone integrations was performed on a grid of $4 \times 4 \times 4$ Monkhorst-Pack k-points using Gaussian smearing of $\sigma = 0.2$ Ry.

Notes and references

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