

# Enthalpies and Elastic Properties of Ni-Co Binary System by *ab initio* Calculations and an Energy Comparison with the CALPHAD Approach

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## Abstract

Enthalpies and elastic properties of the full composition range of Ni-Co binary system with FCC structure were investigated applying Density Functional Theory (DFT). The DFT results on enthalpy were compared with the enthalpies calculated applying the CALPHAD approach. Moreover, the effect of relaxation method, i.e. volume relaxation vs. energy-volume (E-V) curves, in DFT approach on the accuracy of the results of thermodynamic and mechanical properties were studied. It was shown that the results are very close together for the regions in which FCC is stable, but different in FCC-metastable regions.

*Keywords: DFT; ab initio calculations; CALPHAD; Ni-Co alloys; Relaxation method; Mechanical properties*

## 1. Introduction

Ni-Co alloys have been studied by various research groups due to their critical engineering applications. One of the applications of these alloys is as active materials in water electrolysis for hydrogen or oxygen evolution reactions, which is due to their electrocatalytic activity [1-5]. These alloys are also applied in magnetic devices because of their magnetic properties [6, 7]. Ni-Co alloys also exhibit other interesting properties, including good wear resistance, high strength, and high thermal conductivity [8-10].

According to the critical abovementioned applications of Ni-Co alloys, further understanding of this alloy along with providing proper guidance for their future developments seem necessary. Kim et al. studied the effect of alloying elements on the elastic properties of Ni by first-principles calculations [11]. They considered several different elements; however, the study was focused only on dilute solutions. Shang et al. also studied the effect of different alloying elements on the elastic properties of dilute Ni-base solutions considering the effect of temperature applying first-principles calculations [12]. However, there are still several questions need to be answered about the Ni-Co system. The elastic moduli of the full composition range of Ni-Co alloy should be investigated to provide a prediction on its mechanical properties. Moreover, due to the widespread application of the Density Functional Theory (DFT) approach in the study of thermodynamic and mechanical properties of different alloys, it is important to examine the effect of relaxation method on the accuracy of the results. Therefore, it is crucial to establish a

framework for the application of DFT approach in the prediction of different properties of the alloys.

In this paper, Ni-Co binary system was studied in its full composition range applying first-principles calculations. The enthalpy of mixing for FCC crystal structure was calculated using both DFT and the CALculation of PHase Diagrams (CALPHAD) approach and the results were compared. In addition, the elastic properties of the Ni-Co alloys with FCC structure were calculated using the DFT method and the results were compared with the related experimental data. Moreover, two common DFT approaches to calculate the energy and elastic properties were utilized and compared for the Ni-Co binary system to evaluate which approach is more reliable by giving closer results to the experimental data. FCC crystal structure was chosen in this study because it is the stable phase in the most Ni-Co composition range at low temperatures. The differences observed between the results of CALPHAD and DFT approaches were discussed, which can pave the way for their future engineering applications and can enhance the development of more accurate thermodynamic databases. In addition, the comparison between the results of mechanical properties by DFT method in this work and available experimental and computational data in the literature, and discussions of the possible reasons of the differences can greatly facilitate the future engineering applications of DFT to predict the mechanical properties of alloys.

## **2. Computational setup**

The enthalpy of mixing for the whole composition range of the Ni-Co system was calculated applying the DFT and CALPHAD approach. The computational details of each method are explained below.

### **2.1. The CALPHAD approach**

The Gibbs free energy is a characteristic state function which is of great importance since it is minimized at equilibrium under constant temperature and pressure, so it is a key factor to determine the fundamental properties of a material. Interestingly, temperature and pressure are the variables which typically controlled in the experiments. The CALPHAD approach relies on the modeling of Gibbs free energy of each individual phase in a system. Therefore, it has become a powerful tool to predict the properties of a material at a determined condition [13-18].

In this work, the software PANDAT developed by CompuTherm LLC [19] was utilized to calculate the enthalpies of mixing in the Ni-Co binary system. The PanIron thermodynamic database provided by CompuTherm LLC was applied.

### **2.2. First-principles calculations**

The first-principles calculations to study the energy in Ni-Co binary system were performed applying the Vienna ab initio simulation package (VASP) [20, 21]. In order to describe exchange and correlation effects, the generalized gradient approximation (GGA) with the Perdew-Burke-Ernzerhof (PBE) functional was utilized [22, 23]. The projector augmented wave method (PAW)

was applied to describe ion-electron interactions with a cutoff energy of 500 eV [24]. Monkhorst-Pack [25] k-points mesh with density higher than 1000 per-reciprocal-atom was used for the Brillouin zone integration. The energy convergence criterion for atomic relaxation was  $10^{-5}$  eV per atom, while all of the forces on each atom were less than 0.01 meV/Å.

For the calculation of elastic properties in the Ni-Co binary system, cutoff energy and k-points mesh density were increased to 700 eV and 7000 per-reciprocal-atom, respectively, since higher accuracy must be obtained compared to a total energy calculation. Elastic constants of the Ni-Co alloy were calculated by determining the Hessian matrix, which is the matrix of second derivatives of the total energy with respect to the atomic positions. This feature has been implemented in VASP starting from version 5.1. For the calculation of the Hessian matrix, finite differences are utilized, i.e. each ion is slightly displaced in the direction of Cartesian coordinates, and the derivatives of reaction forces with respect to the displacement are calculated [26].

In order to compare two common DFT methods of calculating energy and mechanical properties for Ni-Co system, total energy vs. volume data points (E-V) were fitted on Birch-Murnaghan (BM) equation of state (EOS) [27, 28], from which the equilibrium properties like volume ( $V_0$ ), energy ( $E_0$ ), and bulk modulus ( $B_0$ ) are estimated [12]. For the final calculation of total energies, the tetrahedron method with Blöchl corrections [29] was applied. In the current study, six E-V data points were generated for EOS fitting and the results were compared with the ones obtained using the abovementioned DFT approach, which mainly relies on volume relaxation.

### 3. Results and discussion

The crystal structure of random Ni-Co solid solutions utilized in this work was modeled using Special Quasi-random Structure (SQS) approach [30-34]. It is worth mentioning that Ni-Co alloys and pure Ni possess Face-Centered Cubic (FCC) structure at room temperature, while pure Co has Hexagonal Close-Packed (HCP) structure [35, 36].

The SQS approach is to find the small unit cell periodic structures that possess  $\prod_{k,m}(SQS) \cong \prod_{k,m}(R)$  for as many figures as possible [32, 33], where  $\prod_{k,m}(R)$  is the correlation function of a random alloy.  $\prod_{k,m}(R)$  is defined by  $(2x - 1)^k$  in the  $A_{1-x}B_x$  substitutional binary alloy, where  $x$  is the composition of the alloy and  $k$  is the number of atoms (pair, triplet, quadruplets) considered for the correlation functions. The structures which shows the best agreement with the ideal random alloy will be selected. In this work, we utilized the SQS-generated FCC structure from the work by Wolverton [34]. The SQS-generated FCC unit cell of Ni-Co alloy contained 16 atoms, while the FCC structure of pure Co and Ni contained 4 atoms.

Figure 1 shows the energy-volume (E-V) curve for pure Co, Ni<sub>25</sub>Co<sub>75</sub>, Ni<sub>50</sub>Co<sub>50</sub>, Ni<sub>75</sub>Co<sub>25</sub>, and pure Ni calculated by DFT method. The relaxed crystal structure related to equilibrium volume is also shown in this figure. According to the E-V curves shown in Figure 1, the equilibrium volumes along with their related energies are tabulated in Table 1. As it is seen in Figure 1, for each case of pure Co, Ni<sub>25</sub>Co<sub>75</sub>, Ni<sub>50</sub>Co<sub>50</sub>, Ni<sub>75</sub>Co<sub>25</sub>, and pure Ni, six different volumes were selected and fixed during

relaxation. After the structure was fully relaxed, the energy related to the fixed volume was calculated and all the data points were plotted in one diagram for each composition. The calculated E-V data points were fitted to 3<sup>rd</sup> order Birch-Murnaghan equation of state (BM EOS). As a result of fitting the E-V curves with BM EOS, bulk modulus of each composition can be derived as shown in Table 1.

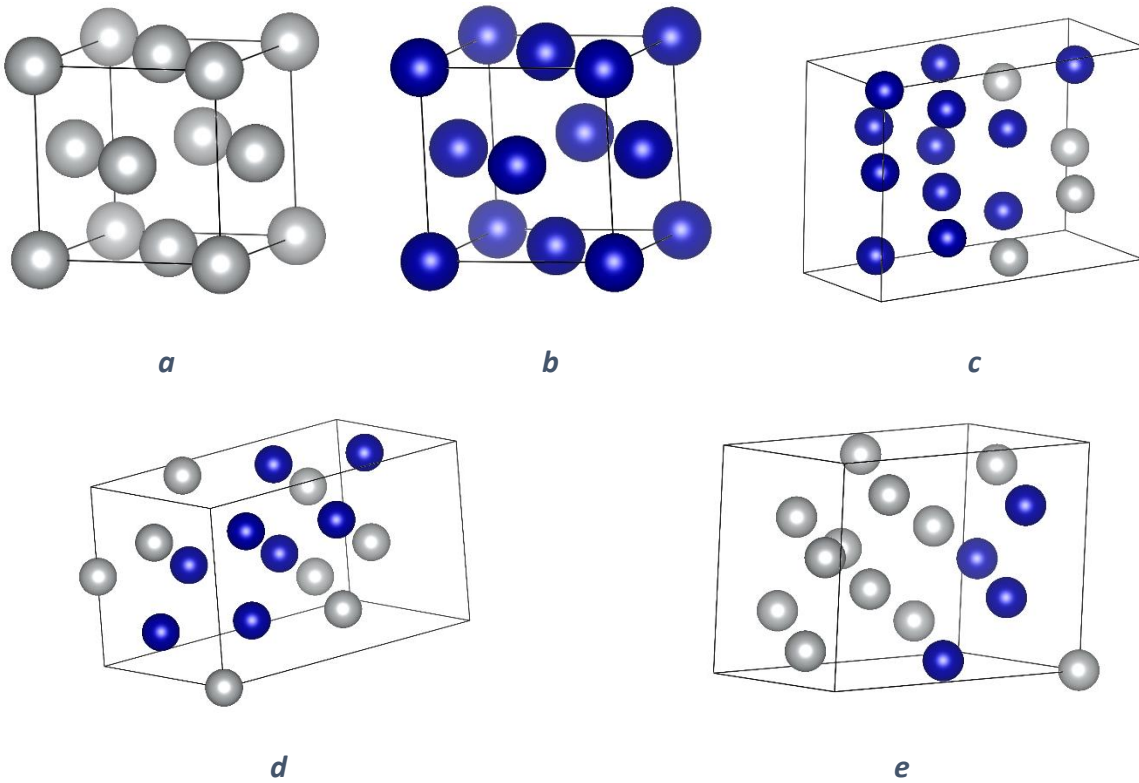
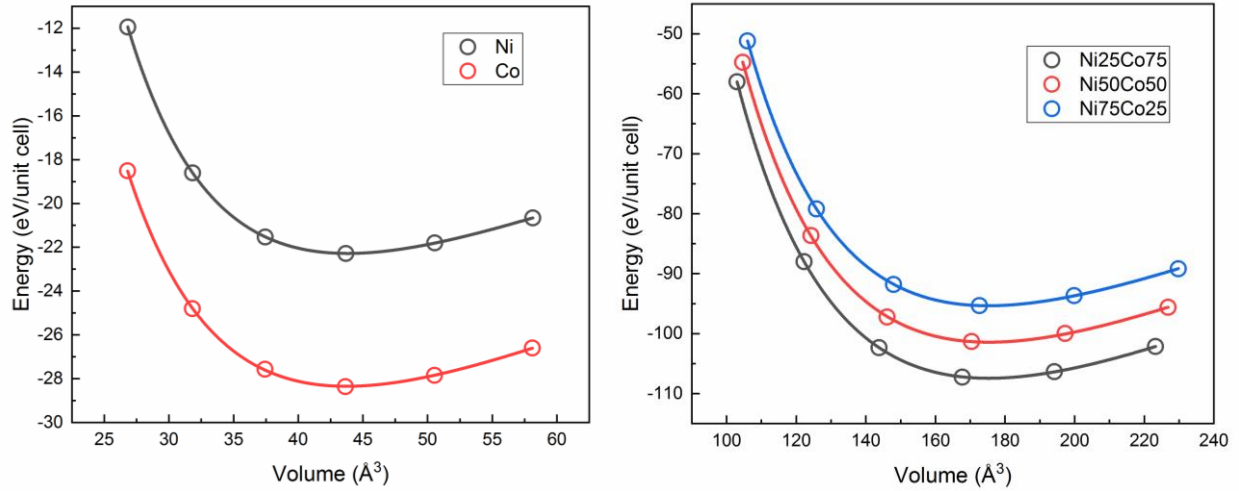


Figure 1. The E-V curves and relaxed crystal structures for equilibrium volumes, a) Pure Ni, b) Pure Co, c) Ni<sub>25</sub>Co<sub>75</sub>, d) Ni<sub>50</sub>Co<sub>50</sub>, e) Ni<sub>75</sub>Co<sub>25</sub>.

Table 1. Equilibrium volume, minimum energy, and bulk modulus derived from E-V curves.

	Co	Ni <sub>25</sub> Co <sub>75</sub>	Ni <sub>50</sub> Co <sub>50</sub>	Ni <sub>75</sub> Co <sub>25</sub>	Ni
Equilibrium Volume ( $V_0\text{-}\text{\AA}^3$ )	43.9405	176.2077	176.3507	176.2340	43.7665
Equilibrium Volume per atom ( $V_0\text{-}\text{\AA}^3$ )	10.9851	11.0130	11.0219	11.0146	10.9416
Minimum Energy ( $E_0\text{-eV}$ )	-28.3388	-107.4686	-101.4422	-95.3463	-22.2820
Minimum Energy per atom ( $E_0\text{-eV}$ )	-7.0847	-6.7168	-6.3401	-5.9591	-5.5705
Minimum Energy per atom ( $E_0\text{-KJ/mole}$ )	-683.5711	-10369.1656	-9787.7051	-9199.5390	-537.4808
Minimum Energy per atom ( $E_0\text{-KJ/mole}$ ) vs. FCC Reference State	0	-1.0583	-1.2736	-1.0698	0
Bulk Modulus ( $B_0\text{-eV/\AA}^3$ )	1.1966	1.2440	1.2265	1.1918	1.1623
Bulk Modulus (GPa)	191.7165	199.3108	196.5070	190.9474	186.2210

Figure 2 shows the comparison of enthalpy of mixing from DFT and CALPHAD approaches for FCC structure of Ni-Co system. The red solid line refers to DFT volume relaxation method and the blue dash line refers to DFT E-V curves method, while the green smooth curve is from the CALPHAD approach. As it is seen in this figure, the Ni-rich side of the diagram shows good match between the results from DFT volume relaxation method and CALPHAD approach. However, by increasing the Co mole fraction from 0.5, discrepancies between the two results appear. In order to explain the reason for this discrepancy, knowing the stability regions in Ni-Co system seems necessary.

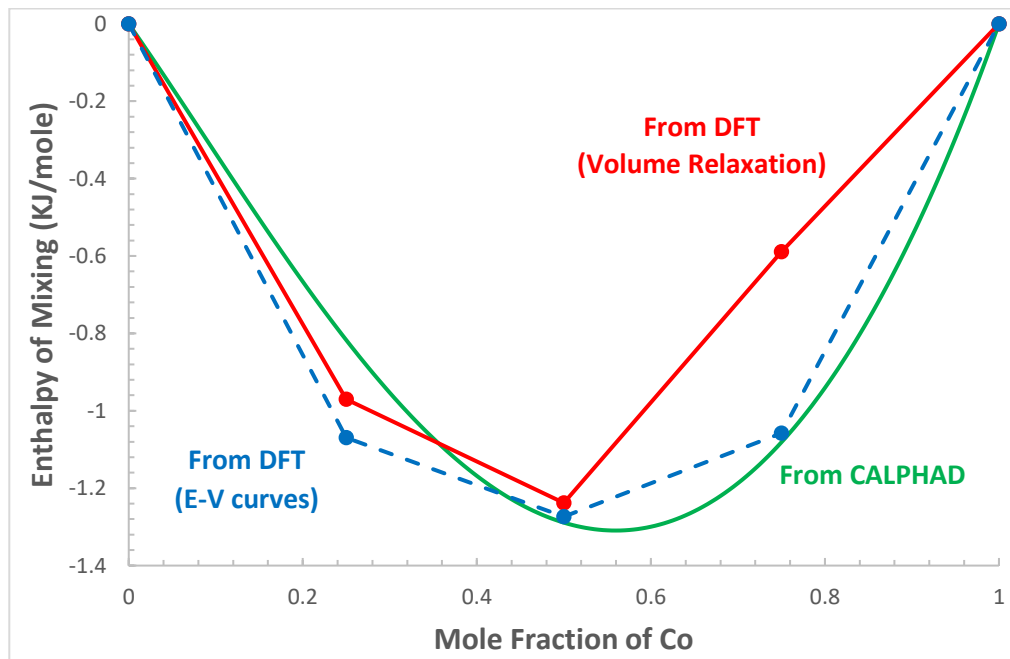


Figure 2. Enthalpy of mixing for FCC structure of Ni-Co system using DFT volume relaxation method, DFT E-V curves, and CALPHAD approach.

Figure 3 shows the phase diagram of Ni-Co system calculated using the CALPHAD approach. Based on this diagram, the FCC structure is the stable phase in Ni-rich side and some parts of Co-rich regions, while the HCP structure is stable at the Co-rich side. As indicated in Figure 2, five data points corresponding to five Ni-Co compositions have been calculated using both DFT methods (volume relaxation and E-V curves). For the Co mole fraction data points of 0, 0.25, and 0.5, good match is seen between DFT volume relaxation method and CALPHAD results, while at the data point 0.75, proper consistency is not seen. According to Figure 3, this composition has HCP structure as a stable phase, while the enthalpy of mixing has been calculated for FCC structure in this work. Therefore, the discrepancy observed at the Co mole fraction of 0.75 data point between DFT volume relaxation method and CALPHAD results is not surprising since a metastable phase is being studied at this region which is FCC. Therefore, possibly due to lack of experimental data to construct the thermodynamic database of the Co-rich side for FCC structure, the energies calculated by the CALPHAD approach for the metastable FCC might not be accurate. In other words, DFT volume relaxation method shows that the enthalpy of metastable FCC at Co-rich side of the Ni-Co system should be lower than what predicted by the CALPHAD approach. This may suggest that the enthalpy of metastable FCC by the CALPHAD approach should shift towards what predicted by DFT volume relaxation method. Nevertheless, the DFT E-V curves method shows a very good agreement with the CALPHAD-calculated enthalpy at Co mole fraction of 0.75, while they are relatively in a good agreement on the Ni-rich side as well.

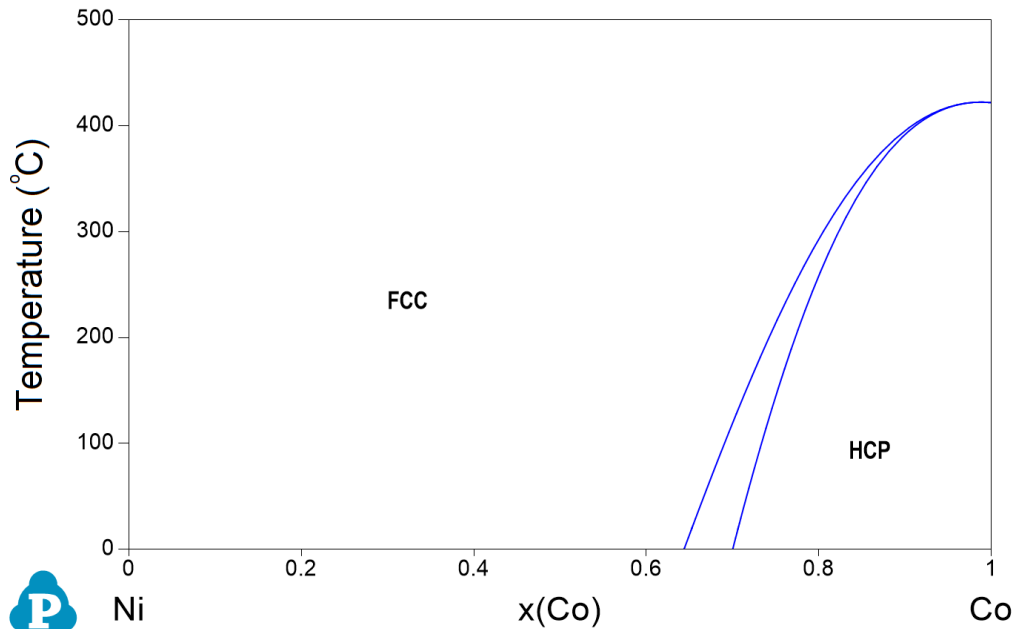


Figure 3. Ni-Co binary alloy phase diagram calculated using Pandat applying the database provided by CompuTherm LLC.

Figure 4 shows unit cell volume ( $\text{\AA}^3/\text{atom}$ ) vs. Co concentration in Ni-Co alloy comparing with experimental data [37-39]. The volumes calculated by both volume relaxation and E-V curves DFT

methods are in good agreement with experimental values. As seen in Figure 2, volume relaxation method underestimates the unit cell volume by about 1% compared to the experimentally measured values. Considering that GGA approximation, which was applied in this work, usually overestimate unit cell volume compared to experimental volumes, we can conclude that E-V curves approach is more proper method to deal with unit cell volume in this system. The volume-composition curve by E-V curves approach also shows good agreement with the Vegard's law (an empirical rule stating that a property of an alloy can be calculated from a linear interpolation of the property values of its constituent elements), while the curve by volume relaxation method shows small deviation. Due to metastability of FCC at the Co-rich side, it is difficult to judge on the DFT-calculated results for that region.

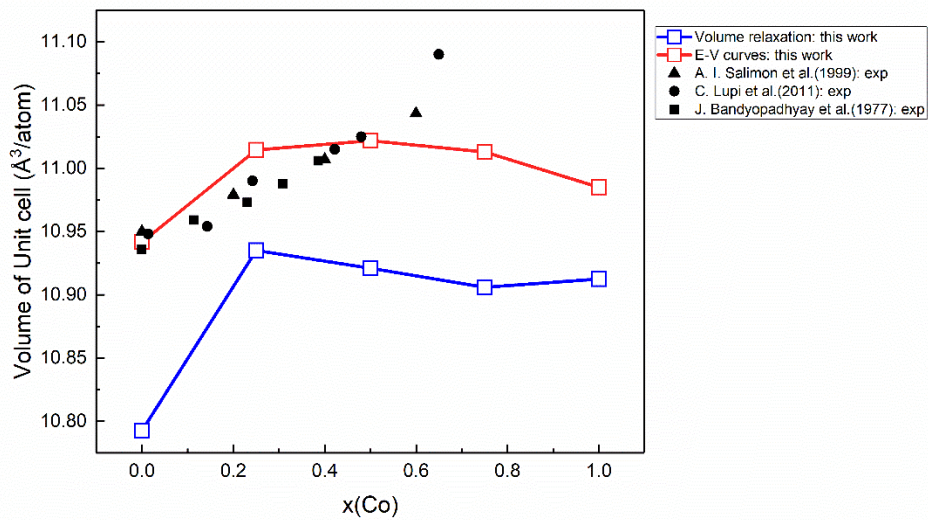


Figure 4. Unit cell volume ( $\text{\AA}^3/\text{atom}$ ) of FCC crystal structure vs. mole fraction of Co in Ni-Co system, from both volume relaxation and E-V curves methods of DFT, along with experimental data.

Figure 5 and Figure 6 show the elastic moduli and Poisson's ratio, respectively, for the Ni-Co system calculated by DFT. The related experimental and computational data are also shown in the diagrams [36, 40-46]. These two diagrams were constructed based on the calculated elastic constants for single crystal FCC, from which the polycrystalline properties were estimated utilizing the Voigt-Reuss-Hill approach [47]. The Voigt approach gives the upper bound of elasticity, the Reuss approach gives the lower bound, and the Hill approach gives average between the Voigt and Reuss approaches.

According to Figure 5, the shear and Young's moduli show relatively good match with the experimental and computational data collected from literature on the Ni-rich side. As it is seen in this figure, the data from other groups are in between upper (Voigt) and lower (Reuss) DFT-calculated boundaries from current work. However, by increasing Co concentration, the DFT results show slight deviation from experimental data. Despite of this deviation, the DFT results are still considered as a good match with experimental data. The first reason is that the

experimental data by Weston et al. [43] for Co-rich side are in a very good agreement with the DFT results from current study for both shear and Young's moduli. The second reason is the differences between presented experimental data from different groups for one composition reveal that the error bars of experimental results have overlap with the results of DFT calculations. The same argument can be applied to consider the bulk modulus from this work also has good agreement with the related results of other groups. As it is seen in Figure 5, the bulk moduli from E-V curves approach are very close to those calculated from volume relaxation method.

For the Poisson's ratio presented in Figure 6 also good match is seen between the DFT-calculated results of this work and the data from other groups. As it is shown in this figure, all of the reported experimental data are in between the upper (Voight) and lower (Reuss) DFT-calculated boundaries from current work.

Regarding the discrepancies observed in the experimental data for some composition ranges, several items including the effects of impurities in the samples tested by different groups, the grain size of the samples, and the differences in measurement and calculation methods should be considered. For example, in the work by Laplanche et al. [42], the grain size of the samples was around 60  $\mu\text{m}$  and they calculated the Poisson's ratio ( $\nu$ ) using the equation below:

$$\nu = -1 + \frac{E}{2G}$$

in which, E and G are Young's and shear moduli, respectively; while in the work by Wu et al. [44], the grain size of the samples was around 35  $\mu\text{m}$  and they measured the Poisson's ratio by ultrasonic techniques. Moreover, Laplanche et al. [42] mentioned that due to opposite influences of texture on Poisson's ratio and bulk modulus (B), their magnitudes might be under or over estimated. In addition, they mentioned that magneto-elastic effects also influenced the room-temperature elastic moduli. The bulk modulus was calculated by the equation below in the paper by Laplanche et al. [42]:

$$B = \frac{E G}{3(3G - E)}$$

The bulk modulus and Poisson's ratio of NiCo alloy were reported 534 GPa and 0.43, respectively, by Laplanche et al. [42], which were not shown in Figure 5 and Figure 6 due to large discrepancy. In addition, the computational results by Liu et al. [46] for bulk modulus in Co-rich region and for Poisson's ratio in Ni-rich region were not shown in the diagrams due to large discrepancies with other presented data. They utilized the Cambridge Serial Total Energy Package (CASTEP) and adopted the GGA with Perdew-Wang91 (PW91) as the exchange-correlation functional. The method they applied in their work was the plane-wave ultrasoft pseudopotential.

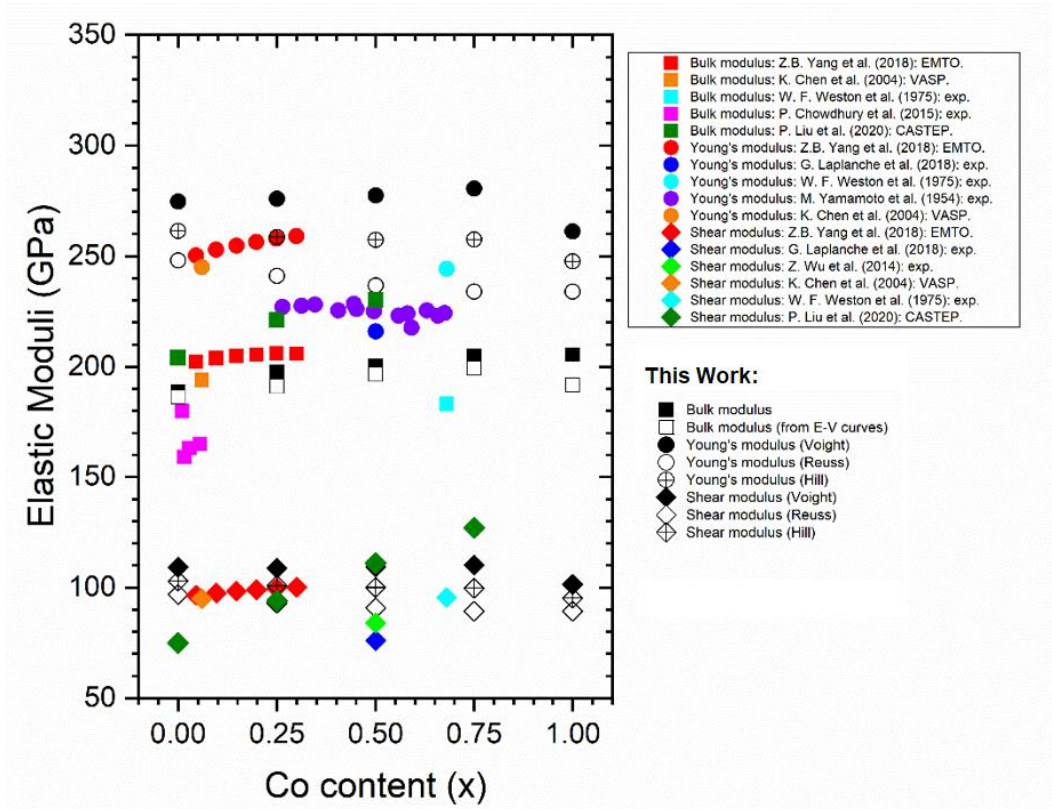


Figure 5. The elastic moduli for Ni-Co system calculated using DFT in comparison with related experimental and computational data.

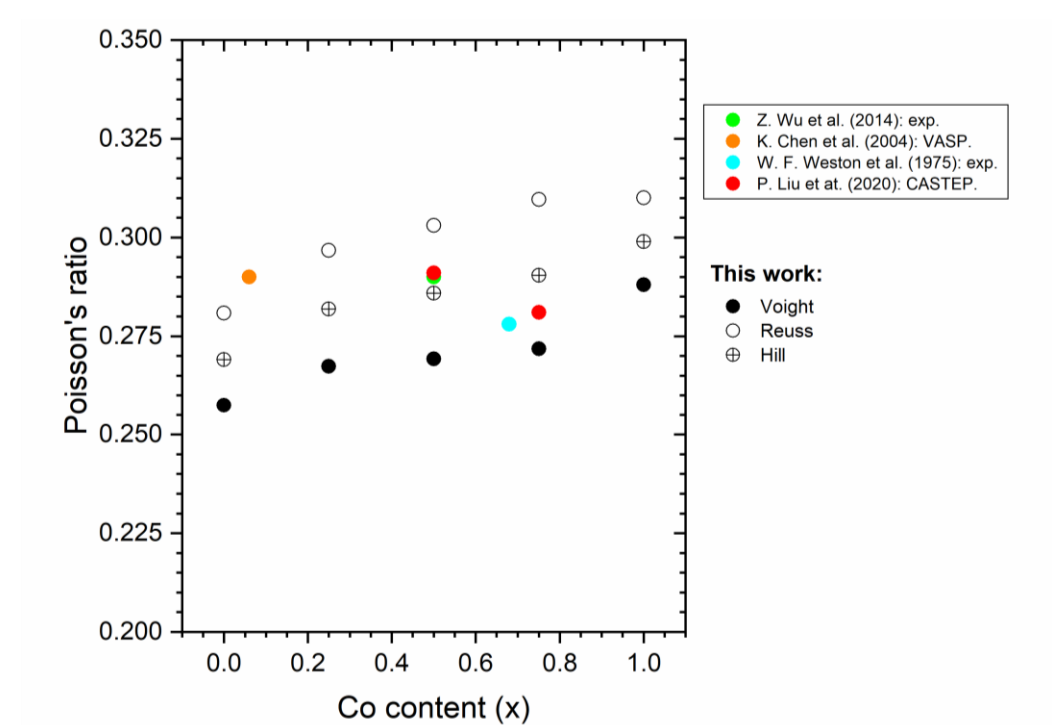


Figure 6. The Poisson's ratio for Ni-Co system calculated using DFT in comparison with related experimental and computational data.

According to Figure 5 and Figure 6, the data by Chen et al. [40] was also calculated by VASP, while they are slightly different from the results of current work. Several reasons can be considered to explain this difference. First, Chen et al. considered separation between the two alloying atoms beyond the second nearest neighbor distance to minimize their interactions [40], while we utilized SQS approach, in which much more nearest neighbors (first, second, third, and even forth) are considered. Second reason is the pseudopotential file, which has been updated since 2004, therefore can provide more accurate results.

#### **4. Conclusions**

The enthalpy and elastic properties of Ni, Ni<sub>75</sub>Co<sub>25</sub>, Ni<sub>50</sub>Co<sub>50</sub>, Ni<sub>25</sub>Co<sub>75</sub>, and Co all with FCC crystal structure were predicted using two different relaxation methods by DFT approach. The enthalpy also calculated for the full composition range of Ni-Co binary system applying the CALPHAD approach. Studies indicated that despite of some small differences, the investigated approaches give similar results. Specifically for the enthalpy of Ni<sub>25</sub>Co<sub>75</sub> composition, some discrepancies observed between the results of volume relaxation method by DFT and that of CALPHAD, while the results from energy-volume (E-V) curves method by DFT showed a very good match with the results from CALPHAD approach. It was explained that since FCC is metastable at Co-rich side of Ni-Co system, the enthalpies predicted by the CALPHAD approach for this region might not be accurate. Overall, this work showed that the DFT method along with SQS approach could provide relatively reliable predictions for both energy and mechanical properties in Ni-Co system. This study can pave the way for more practical applications of DFT to predict thermodynamic and mechanical properties of different alloys, especially multi-component alloys.

#### **Acknowledgement and Disclaimer**

The authors acknowledge the Extreme Science and Engineering Discovery Environment (XSEDE) and National Supercomputer Center in Sweden (NSC) for providing the computing resources. This material is based upon work supported by the Department of Energy under Award Number **DE-FE0030585**. The authors would like to thank the support and guidance from the DOE National Energy Technology Laboratory program manager, Maria M. Reidpath. This paper was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

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