Ab-initio Simulations of Ni and Ni$_{0.5}$Cu$_{0.5}$ Generalized Stacking Fault Energies

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Abstract. We performed ab-initio calculations based on density functional theory (DFT) for obtaining the generalized stacking fault energies (GSFEs) and elastic moduli of Cu, magnetic and non-magnetic Ni and Ni$_{0.5}$Cu$_{0.5}$ alloy. We have studied the effect of magnetism on the elastic constants and GSFEs in 50% Cu doped Ni alloy. The GSFEs and elastic constants show a decrease upon Cu doping in agreement with the trends in theoretical and experimental results for Ni-rich alloy of Ni-Cu. The Rice criteria [1] analysis showed that adding Cu to Ni reduces the ductility of Ni which may lead to an increase in the strength of alloy compared to pure Cu and Ni.

INTRODUCTION

It is well known that metals have stacking faults due to lattice dislocations, which can be either partial or complete which affect their aging performance. Dislocations may cause plastic deformation due to their movement along the slip planes in crystal lattices. The effect of dislocations on the deformation behavior can be characterized through an understanding of the GSFEs, which are difficult to obtain experimentally but possible theoretically for any alloy composition of interest. GSFE’s in combination with the elastic constants can help to evaluate and understand the mechanical properties of metals and metal alloys; especially the role and percentage of doping on these properties.

With this motivation, we have calculated the generalized stacking fault energies and elastic constants of Cu, Ni and Ni$_{0.5}$Cu$_{0.5}$. In Ni and Ni-rich alloys, GSFEs and ductility have been studied to understand their mechanical behavior [2, 3, 4]. Theoretical studies on Ni and Ni based alloys by Siegel [2], report a reduction of 21 and 6% in the intrinsic stacking fault energy ($\gamma_{sf}$) and unstable stacking fault energy, ($\gamma_{usf}$) respectively for Ni-rich (less than 20 at.% Cu) alloy in comparison with Ni. Experimental studies by Gallagher [5] report that inclusion of transition metal in Ni shows a significant reduction in stacking fault energies. Ductility of materials is related with $\gamma_{usf}$ [1], and a lower value of $\gamma_{usf}$ results in higher ductility which has implications on the strength of materials.

COMPUTATIONAL METHODOLOGY

Ab-initio calculations based on density functional theory (DFT) were performed using the Vienna Ab initio Simulation Package (VASP) [6] to optimize the lattice parameter of the fcc structure of Ni and Ni$_{0.5}$Cu$_{0.5}$. We used the PAW potential [7, 8] to model the electron-ion interactions and the exchange-correlation functional as parameterized by Perdew, Burke, and Ernzerhof (PBE) [9]. Based on the energy and k-points convergence studies, a plane wave basis with energy cutoff of 600 eV and a Monkhorst-Pack k-point grid [10] of 11x11x11 were used for both spin and non-spin polarized calculations of Ni and Ni$_{0.5}$Cu$_{0.5}$. For GSFEs calculations, we have used a plane wave basis energy cutoff as above and k-point grid of 5x3x1. The total energy is converged within 1 μeV and the forces on each atom to 1 meV/Å. We have used a 2 × 3 unitcell for Ni and Ni$_{0.5}$Cu$_{0.5}$, with periodicity in the x- and y-directions and vacuum spacing of 15 Å in the z-direction to avoid interactions between periodic images of the crystal slabs for obtaining the GSFEs. Crystal dislocations have been modeled by sliding half of the total number of layers in the crystal slab with {111} plane orientation along the <110> and <112> directions of the sliding plane.
The GSFE calculations are performed using 10 layers based on the observations in earlier studies [11]. The structure of the perfect crystal slabs and that with stacking faults for Ni$_{0.5}$Cu$_{0.5}$ are shown in Fig. 1. (a)-(c).

FIGURE 1. Structure of the perfect crystal of (a) Ni$_{0.5}$Cu$_{0.5}$, and with dislocation for (b) 0.5$b$ and (c) 1$b$ displacement along <110> and <112> directions., where $b$ is the Burgers vector given as $b = a \langle 112 \rangle / 6$

To calculate the elastic moduli for Ni and Ni$_{0.5}$Cu$_{0.5}$ alloys, we adopted the methodology described by Ravindran et al [12] that uses the energy-strain relation. We have applied a small deformation strain in the range of $-0.03 \leq \delta \leq 0.03$ with a step of $\pm 0.01$ within the elastic limits. In cubic system, there are three independent elastic constants i.e. $C_{11}$, $C_{12}$ and $C_{44}$. We used three different distortion matrices as given in [12] to determine $C_{11}$, $C_{12}$ and $C_{44}$, and the bulk modulus based on these as; $B=(C_{11}+2C_{12})/3$.

RESULTS AND DISCUSSION

The spin-polarized calculations of the structural optimization of Ni gave the lattice constant as 3.518 Å, which is in good agreement with the experimental value of 3.52 Å [13, 14]. The lattice parameter of 3.569 Å for Ni$_{0.5}$Cu$_{0.5}$ shows agreement with the experimental value of 3.57 Å [15]. 50% Cu dopant has expanded the Ni lattice by 5%. We list the optimized lattice parameters and elastic constants in Table 1, for Ni (magnetic and non-magnetic), Ni$_{0.5}$Cu$_{0.5}$ (magnetic and non-magnetic) and Cu. Our calculated elastic constants for Ni are in good agreement with the experimental values [16]. For Ni$_{0.5}$Cu$_{0.5}$, calculated elastic moduli are within the error range of experimental values for Ni$_{53.8}$Cu$_{46.2}$ [17]. The values of elastic moduli and bulk modulus (B) of Ni are larger than Ni$_{0.5}$Cu$_{0.5}$. It has been observed that the values of elastic constants decrease significantly as the concentration of Cu increases in Ni [2, 5]. This decrease in the elastic constants of Cu doped Ni implies a decrease in stiffness rendering the alloy prone to fracture under applied stress in comparison with pure Cu and Ni.
**TABLE 1.** Calculated lattice parameters and elastic constants for Ni, Cu and Ni$_{0.5}$Cu$_{0.5}$.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Ni</th>
<th>Ni$<em>{0.5}$Cu$</em>{0.5}$</th>
<th>Cu</th>
</tr>
</thead>
<tbody>
<tr>
<td>C$_{11}$ (GPa)</td>
<td>275.82</td>
<td>253 [16]</td>
<td>203.78</td>
</tr>
<tr>
<td>C$_{12}$ (GPa)</td>
<td>159.22</td>
<td>158 [16]</td>
<td>148.95</td>
</tr>
<tr>
<td>C$_{44}$ (GPa)</td>
<td>131.84</td>
<td>122 [16]</td>
<td>100.84</td>
</tr>
<tr>
<td>B (GPa)</td>
<td>198.09</td>
<td>189.67</td>
<td>167.23</td>
</tr>
</tbody>
</table>

We have calculated the GSFE values for Cu, Ni and Ni$_{0.5}$Cu$_{0.5}$ at special points $G_1(0.25b)$, $G_2(0.5b)$, $G_3(0.75b)$, $G(1b)$, $T_1(0.125b)$, and $T(0.25b)$ and listed them in Table 2. The value in parenthesis denotes the amount of shift given to the perfect crystal structure. For Ni, our $\gamma_{suf}$ of 143.74 mJ/m$^2$ is in agreement with the theoretical values [19-21] and overestimated from the experimental value of 125-128 mJ/m$^2$ [13, 14]. The $\gamma_{suf}$ of 228.24 mJ/m$^2$ is underestimated compared to the reported theoretical values [2-4, 19-21]. For magnetic Ni$_{0.5}$Cu$_{0.5}$, the calculated value of $\gamma_{suf}$ is 128.56 mJ/m$^2$ and $\gamma_{suf}$ is 233.23 mJ/m$^2$ which are greater than the values obtained by non-magnetic calculations. Compared to the $\gamma_{suf}$ in non-magnetic Ni, the magnetic Ni shows a better agreement with the experimental results [13, 14]. The decrease in GSFE increases the stacking fault width (SFW), which enable insight into the dynamics of several nucleating and interacting dislocations and helps predict the plastic deformation behavior in materials.

**TABLE 2.** The calculated stacking fault energies (mJ/m$^2$) in Cu, magnetic and non-magnetic Ni, Ni$_{0.5}$Cu$_{0.5}$, where, G and G$_2$ are the intrinsic and unstable stacking faults.

<table>
<thead>
<tr>
<th>Shift</th>
<th>Ni</th>
<th>Ni$<em>{0.5}$Cu$</em>{0.5}$</th>
<th>Cu</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Non-magnetic</td>
<td>Magnetic</td>
<td>Non-magnetic</td>
</tr>
<tr>
<td>A(0)</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>G1(0.25)</td>
<td>132.83</td>
<td>146.59</td>
<td>118.77</td>
</tr>
<tr>
<td>G2(0.5)</td>
<td>263.37</td>
<td>228.24</td>
<td>229.99</td>
</tr>
<tr>
<td>G3(0.75)</td>
<td>228.25</td>
<td>244.01</td>
<td>176.39</td>
</tr>
<tr>
<td>G(1.0)</td>
<td>143.79</td>
<td>143.74</td>
<td>69.02</td>
</tr>
<tr>
<td></td>
<td>139.01 [21]</td>
<td>134 [20]</td>
<td>69.02</td>
</tr>
<tr>
<td>T1(0.125)</td>
<td>415.33</td>
<td>465.02</td>
<td>284.74</td>
</tr>
<tr>
<td>T(0.25)</td>
<td>704.70</td>
<td>800.69</td>
<td>684.67</td>
</tr>
</tbody>
</table>

To analyze the influence of alloying elements on Ni we use Rice criterion [1] that defines ductility as $D = \frac{0.3\gamma_{surf}}{\gamma_{suf}}$, where $\gamma_{surf}$ is surface energy. The Rice criterion characterizes materials to be ductile if D>1. Thus, a hardened material would have a lower value of the ductility parameter D, whereas ductile materials a larger value. The value of D for Cu and magnetic Ni is 2.53 and that for Ni$_{0.5}$Cu$_{0.5}$ alloy it is 1.59. The ductility of Ni$_{0.5}$Cu$_{0.5}$ is lower than that of the Ni-rich Ni-Cu alloy. Our results show that Cu dopant reduces the GSFEs as well as the ductility of Ni.

**CONCLUSION**

The elastic constants and bulk modulus decrease with the addition of Cu dopant in Ni which agrees well with the experimental results and follows the trends in literature. Cu has the smallest GSFE and Ni has the largest GSFE although they exhibit the same ductility value. Doping with Cu causes a decrease in both the GSFEs as well as ductility of the Ni-alloy in comparison with Cu and Ni.
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REFERENCES