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Contribution of stacking fault in lowering the theoretical density of nickel

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ABSTRACT

It has been shown with the help of first-principle based calculations that the occurrence of stacking fault (SF) changes the density of nickel. Calculations, based upon a twelve {1 1 1}-plane supercell of face-centered-cubic (*fcc*) nickel show that the stacking fault energy in the case of "conventional" stacking is higher by ~2 mJ/m^2 than that of the supercell having an appropriate dilation along the fault-plane normal. The {1 1 1}-type stacking fault energy of *fcc*-Ni, 136.683 mJ/m^2, has been calculated using 4.09746×10^5 mm^2/mm^3 SF density, which has resulted in the decrease in the bulk density of *fcc*-Ni by 0.0895%. This approach of relaxation of a structure with stacking faults along the plane normal may be extended to calculate more accurate generalized stacking fault and to measure the lattice distortion due to various values of defect-densities.

1. Introduction

It is long known that crystal defects, which are invariably present even in high purity metal, are responsible for the difference between the measured and the theoretical density of a material [1]. In principle, the change in overall volume, arising from the distortion produced by the defects is reflected in the difference in densities. As per the continuum theory of elasticity, the volume change is measured from the summation of principal components of the strain tensor. However, the inability of this continuum crystal elasticity to describe the lattice distortion in the proximity of a defect renders it ineffective for making an accurate estimate of this distortion.

Although, density functional theory (DFT) based ab initio calculations are able to solve a wide range of structural problems, careful selection of several computational parameters is required to ensure the efficacy of the calculation. Proper choice of exchange correlation functional, *k*-mesh for Brillouin zone integration, cutoff for plane wave and kinetic energy are important in achieving the desired accuracy for pseudo-potential and for projector augmented wave (PAW) based methods. Moreover, spin-polarized calculation may be necessary for the elements with electrons in *d*- & *f*-shell. Also, depending upon the preference for either precise measurement of stress or total energy, typical methods for treating the partial occupancies for band structure calculation should be chosen. For example, the linear tetrahedron method with Blöchl [2] correction formula is required for obtaining high precision in the calculation of total energy.

A way to assess the significance of a defect is to measure the energy associated with it. In the ab initio based modeling this is usually done by calculating the difference in energies associated with the perfect structure and the structure with the relevant defect. Ideally, this should ideally be done through the comparison of the energies of a perfect structure and that of an infinitely large structure with the desired defect. However, it is a common practice in the ab initio packages to use periodic boundary condition (PBC), where a finite size supercell is repeated infinitely, leading to the calculation of energy associated with a typical defect density rather than that of single defect. Since, the PBC creates a situation, where the original defect in the supercell interacts with its images, some contribution from this in the total energy calculation is unavoidable depending upon the field associated with the defect. This compels one to consider a large supercell so that defect and its image, when repeated due to PBC are separated by a distance that is long enough to reduce the contribution in the total energy below a certain level of accuracy. Hence, there is always a tradeoff between the requirement of a large supercell to achieve a low defect density and of lowering the computation cost by minimizing the number of atoms. To optimize the number of atoms in the supercell and the desired accuracy, maximum possible distance should be considered in one direction between the defect and its image but minimum possible distance in two other directions, where periodicity of the bulk would be maintained when repeated using PBC. In this report, a perspective for computing the lattice dilation due to the stacking fault (SF) has been discussed, and the

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same is applied for the case of pure nickel. This has brought out a general methodology for calculating the contribution of a certain defect density in changing the volume of the supercell vis-à-vis the theoretical density of the material.

2. Computational methodology

Spin-polarized, plane-wave based first principles calculations have been employed in the frame work of density functional theory within the generalized-gradient-approximation (GGA), parameterized by Perdew–Burke–Ernzerhof (PBE) [3,4] scheme, as implemented in the Vienna ab initio simulation package (VASP 5.2) program [5–7]. The spin-polarized, ion–electron interaction has been incorporated using PAW potentials [8,9] as supplied in the VASP database.

In order to achieve a precision better than 10^{-7} eV per atom in the calculation of total energy, the optimized cutoff for plane wave and kinetic energy were taken to be 1050 eV and 540 eV, respectively, in order to accurately calculate the *small energy differences*. These optimized cutoffs were about 1.5 times the default values in the corresponding PAW potential. Brillouin zone integration has been done using corrected tetrahedron method [2] with Γ-centered k-meshes of $23 \times 23 \times 23$ for optimizing the unit cell of nickel and $23 \times 13 \times 3$ k-meshes for the static energy calculations of twelve (111)-planes bulk and SF-structures.

To optimize the lattice parameter of face-centered-cubic (*fcc*) Ni, unit cells with nine different lattice parameters around the tentative optimum value have been created. Static energy calculations on these structures have been carried out using VASP. Equation of state, as suggested by Murnaghan [10] and Birch [11], henceforth called *BM3*, has been used to obtain minimum values of energy (E_0) and volume (V_0). The *BM3*-fitted V_0, so obtained, has been used as an initial value for further optimization over volume in order to achieve true minimum in the energy. This optimized lattice parameter has been used for constructing the supercells, which are used for calculating the total energies of bulk and of SF.

Input structure comprising 24 atoms has been created by stacking 12 (111)-planes having three orthogonal vectors in directions, $[1\bar{1}0]$, $[11\bar{2}]$ and [111]. When viewed from a $\langle 111 \rangle$ direction, atomic arrangements on the (111)-type *ABC* planes of Ni appear like the arrangement depicted in Fig. 1, which has been illustrated using XCRYSDEN [12]. Hence, based on the optimized lattice parameter, the dimensions of the supercell are set to be one (110)-plane spacing in the x-direction ($[1\bar{1}0]$), $d_{(110)}$, two (112)-plane spacing in the y-direction ($[11\bar{2}]$), $2d_{(112)}$, and twelve (111)-plane spacing in the z-direction ([111]), $12d_{(111)}$. This 24-atom supercell has been the basis of calculating the energies of both the bulk and the structure containing the SF. The latter structure has been achieved by tilting z-vector, as suggested in the literature [13,14].

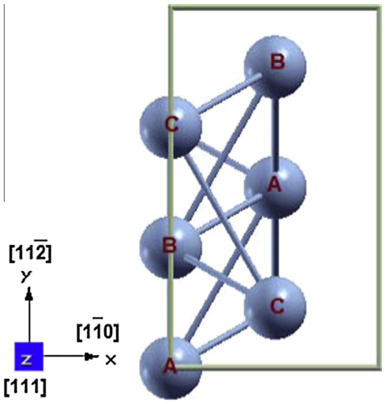

Fig. 1. Positions of atoms on the (111) planes of Ni within the supercell when viewed from [111] directions. A's, B's and C's correspond to positions of atoms in A-plane, B-plane and C-plane, respectively.

Apart from calculating cohesive energies of the bulk and the *SF containing structures* on the aforementioned structures, static energy calculations have also been carried out on five different structures, having variation only in z-dimension, as depicted in Fig. 2. Here the z-dimension corresponding to "position 1" for both, bulk and SF, corresponds to 12 times (111) plane spacing of the optimized Ni-lattice.

3. Results and discussion

For various lattice parameters, energies of *fcc*-Ni unit cells, each comprising 4 atoms, have been calculated and the same have been plotted against their volumes in Fig. 3. Based on the *BM3*-fitted minimum volume, corresponding to the minimum energy, optimized lattice parameter of *fcc*-Ni has been calculated to be 352.26124×10^{-3} nm. Cohesive energies of Bulk and SF, abbreviated as, TE_B and TE_{SF}, respectively, for various z-dimensions, as illustrated in Fig. 2, have been given in Table 1. Fittings of these energies against their respective volumes using *BM3*, as illustrated in Fig. 4, have given the minimum energies, E_0's, corresponding to the volumes, V_0's, which are listed in Table 2 along with the corresponding goodness of fit data. Fittings of Bulk and SF data in Fig. 4 show that unlike the energy-well of *bulk structures*, the minimum of the energy-well of *SF-containing structures* is significantly away from "position 1". Value of the z-dimension corresponding to the minimum of *SF-containing structure*, Z_{SF}, is obtained as follows.

$$Z_{SF}\ (\text{in nm}) = \{V_0 \text{ corresponding to energy-well of SF}\}/\{\text{Area of the (111) plane}\}$$

$$= \{V_0 \text{ corresponding to energy-well of SF}\}/\{d_{(110)} \times 2d_{(112)}\}$$

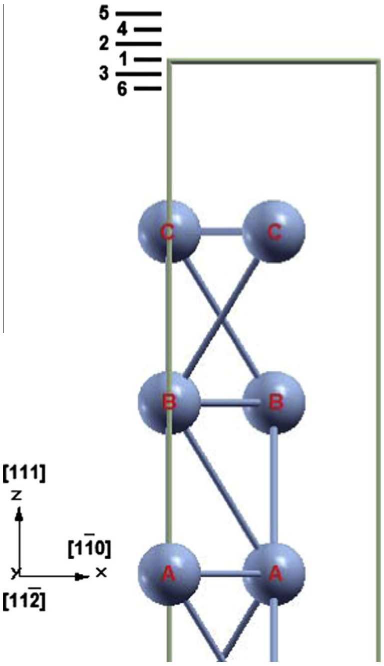

Fig. 2. Atoms on the top three (111) type ABC planes within the supercell are shown above. While position 1 is based upon the fully relaxed lattice parameter, relative other five different z-dimensions of supercells, which are given in Table 1, are indicated at the top using numerics "2" to "6".