EP04

Boron Distribution Behaviors in bcc Iron

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Since 1930's, it has been well established that the hardenability and the corrosion-erosion resistant properties of steels can be greatly enhanced by the trace addition of boron to steels. Recent experiments showed that this effect is related to the thermal diffusion and segregation of boron to the surface and the grain boundaries in the cooling process. Hence, the understanding of boron distribution behavior is essential to trace back the effect of boron addition and its incorporation mechanism with the host material. To model the microstructure of boron distribution in bcc iron, we employed the spin-polarized density functional theory (SDFT) using the full-potential linearized augmented plane wave (FLAPW) band method. For the treatment of exchange-correlation energy, we used the generalized gradient approximation (GGA96). The formation energies for both interstitial and substitutional boron impurities in the 2 × 2 × 7 Fe slab-supercell were calculated. We found that boron impurities on the surface are most stable as compared to the impurities in the sub-surface positions, which is in good agreement with the experiments. In addition we found that both the substitutional and the interstitial positioning of boron impurities are energetically comparable each other. These results are compared with the distribution behaviors of C and N impurities in the same Fe slab-supercell matrices.

EP05

Magnetic Properties of Transition Metals Doped NiO

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ABINIT program package[1] based on Density Functional Theory (DFT) within the Generalized Gradient Approximation (GGA) and plane wave basis set are used to calculate the magnetic propert of transition metal (A = Fe, Mn) doped NiO. It found that the magnetic propert of $Ni1-_xA_xO$ were changed from anti-ferromagnetic (pure NiO) to ferromagnetism. Increasing the concentrations of A, the magnetization of A doped NiO increased ($Ni_{31}FeO_{32}$ = 57.27 μB, $Ni_{30}Fe_2O_{32}$ = 67.95 μB, $Ni_{29}Fe_3O_{32}$ = 69.96 μB, $Ni_{31}MnO_{32}$ = 66.69 μB, $Ni_{30}Mn_2O_{32}$ = 69.59 μB and $Ni_{29}Mn_3O_{32}$ = 72.42 μB).

REFERENCES

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