

New Materials for Spintronics by Grain Boundary Engineering

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We present a systematic ab initio study of segregation of 12 non-magnetic sp-impurities (Al, Si, P, S, Ga, Ge, As, Se, In, Sn, Sb and Te) at $\Sigma 5(210)$ grain boundary (GB) and (210) free surface (FS) in fcc ferromagnetic cobalt and nickel and analyze their effect on structure, magnetic and mechanical properties. We determine the preferred segregation sites at the $\Sigma 5(210)$ GB for the sp-impurities studied, their segregation enthalpies and strengthening/embrittling energies with their decomposition into the chemical and mechanical components. We find interstitially segregated Si as a GB cohesion enhancer, substitutionally segregated Al and interstitially segregated P with none or minimum strengthening effect and interstitially segregated S, Ge, As, Se and substitutionally segregated Ga, In, Sn, Sb and Te as GB embrittlers. In nickel, most of the above impurities nearly kill or substantially reduce the magnetic moments at the FS and, when segregating interstitially (i.e. Si, P, S, Ge, As, Se), also at the GB so that they provide atomically thin magnetically dead layers which may be very desirable in spintronics. Reduction of magnetic moments at the $\Sigma 5(210)$ GB in fcc ferromagnetic cobalt is, in absolute values, very similar to that in nickel. However, as the magnetic moment in bulk cobalt is higher, we do not observe magnetically dead layers here. It turns out that by focused impurity segregation we can generate atomically thin magnetic layers with tailored magnetization, which can contribute to a new development of technologically important materials. Most of our results are theoretical predictions and we hope that they may motivate experimentalists to conduct new investigations in this field.