

Abstract Submitted
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Rationale for contrasting phonon confinement and interface localization effect in FeAg and FeCr multilayers¹ SAMPYO HONG, TALAT RAHMAN, University of Central Florida — We have performed density functional theory based calculations to investigate the propensity for formation of FeAg and FeCr multilayers. A perfect lattice match between Fe and Ag layers at the FeAg interface was obtained by modeling 45rotated Ag(100) layers epitaxially on bcc Fe(100). In comparison, the FeCr interface was modeled by epitaxial layers of bcc Fe(100) and Cr(100). In FeAg, we find the signature peak of Fe bulk phonons (35 meV) to be substantially diminished and the low energy peaks to be remarkably enhanced, in qualitative agreement with experiment [1]. In contrast, the phonon density of state in the FeCr multilayers do not show any outstanding feature except a slight decrease in the 35 meV peak for the Fe layer at the interface, as compared to that of the middle Fe layer in excellent agreement with experiment [2]. The magnetic moment of the interfacial Fe atoms is larger than those Fe atoms in other layers, as a result of charge transfer from Fe to Ag at the interface. As compared to the middle layers, more spin-up and less spin-down states are occupied at the interface in such a way that Fe donates a large number of spin-down electrons to Ag but receives only a few spin-up electrons from the latter because of the almost fully occupied Ag d-band. [1] B. Roldan Cuenya et al., to be published. [2] Roldan et al, Phys. Rev. B 77, 165410 (2008).

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