Electronic Structure of Random Alloys

CHAD WAXLER, BYOUNG-HAK LEE, Department of Physics, Texas State University at San Marcos, XAVIER CARTOIXÀ, Departament d’Enginyeria Electrònica, Universitat Autònoma de Barcelona — We present a theoretical investigation of the evolution of the electronic properties of the random alloys as they undergo a transition from one pure crystal to another. For random substitutional alloys the Bloch wavevector is not a good quantum number due to the lack of translational invariance. In spite of this obvious fact the conventional methods used for random alloys calculations, e.g., Virtual Crystal Approximation and Coherent Potential Approximation, assume a medium that pertains the same symmetries of the parent compounds. The question we ask is how well the band structures from such effective medium theories agree with the real electronic structures. We address this issue using direct simulations of randomly distributed (Al,Ga)As and (In,Ga)P atom structures.