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Ab-initio calculations of phonon properties for the Nb-Mo alloy using the virtual crystal approximation O. DE LA PEÑA-SEAMAN, R. DE COSS, Department of Applied Physics, Cinvestav-Merida, Mexico, R. HEID, K.-P. BOHNEN, Institut fuer Festkoerperphysik, Forschungszentrum Karlsruhe, Germany — We have studied the structural, electronic, and lattice dynamic properties of the $Nb_{1-x}Mo_x$ alloy within the framework of the density functional perturbation theory, using the mixed-basis pseudopotential method and the virtual crystal approximation (VCA) for modeling the alloy. The calculations were performed for both LDA and GGA *xc*-functional approximations. The structural parameters were optimized via the total-energy method for the whole range of Mo-concentration ($0 \leq x \leq 1$). The electronic properties were analyzed in terms of the electronic topological transitions (ETT) in the Fermi surface. The calculated phonon dispersion curves for the different Mo-concentrations are in very good agreement with experimental data reported in the literature. We find that LDA results are in general higher in frequency than GGA. The evolution of the Kohn anomaly in the ΓH direction observed experimentally in the Nb-Mo alloy is well reproduced by the VCA calculations. Thus, we have shown that the virtual crystal approximation as implemented in the present work is useful for the study of random intermetallic alloys where the alloying elements are adjacent in the periodic table. This research was supported by CONACYT, Mexico under Grant No. 43830-F.

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