Abstract Submitted
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First principles molecular dynamics simulations of the static, dynamic and electronic properties of the liquid silver-tin alloy[1] LAZARO CALDERIN, The Pennsylvania State University, PA, USA, DAVID GONZALEZ, LUIS E. GONZALEZ, Universidad de Valladolid, Valladolid, Spain — We report an ab-initio molecular dynamics study of several structural and dynamic properties of the liquid Ag-Sn alloy at three concentrations and a temperature of 1273 K. The calculated structural results show good agreement with the available experimental data and accurately reproduce the measured total static structure factors [1]. The heterocoordinating tendencies in the alloy have been analyzed in terms of some short range order parameters. As for the dynamical properties, the single particle dynamics in the liquid alloy has been studied by evaluating several velocity correlation functions and the associated diffusion coefficients. Results are also reported for other transport coefficients, such as the adiabatic sound velocities and shear viscosities. Finally, from the spectra of the longitudinal current correlation functions, the longitudinal dispersion curves have been computed. [1] I Kaban, W Hoyer, A Ilinski, O Slukhovskii and S Slyusarenko, J. Non-Cryst. Solids, 331, 254-262 (2003)

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