Ab Initio MD Modeling of the Structure and Thermodynamic Properties of Liquid Al-Ni-Ce Alloys

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Abstract. Ab initio molecular dynamics simulations were performed to study the structure and thermodynamic properties of liquid Al, Ni, Ce, binary Al_3Ni and Al_3Ce melts, and the Al-rich ternary melt $Al_3(Ni_{0.5}Ce_{0.5})$ at 1823 K (1550 °C). The reliability of the computational approach was confirmed by agreement between calculated and available experimental structure factors for liquid Al, Ni, and Al_3Ni. Structural factors of binary and ternary melts revealed systematic changes in short-range order caused by alloying additions. The ternary melt exhibited features similar to liquid Al_3Ce, indicating an important role of Ce in the formation of local atomic structure. Negative enthalpies of mixing of the investigated liquid alloys indicate strong chemical interaction. Calculated self-diffusion coefficients showed reduced atomic mobility in binary and ternary melts compared with pure liquid aluminum.