Turkish Journal

of

Physics

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Turkish Journal of Physics

The Structure of Liquid Alloys with Chemical Short Range Order

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Abstract: We present a study of the structural properties of liquid binary alloys with chemical short range order starting from the effective interatomic pair potentials. The interatomic pair potentials are derived using the second order pseudopotential theory and the static structure is obtained using the modified hypernetted chain approximation. The partial structure factors $S_{ij}(q)$ and the concentration - fluctuation structure factor $S_{cc}(q)$ are calculated to analize the ordering tendencies in a binary alloy. In this work, liquid Li-Mg alloy is studied as a test case. The agreement between theory and experiment is quite good. We conclude that the structural properties of liquid alloys with chemical short range order, may be studied successfully by employing analytical Pettifor-Ward pair potentials.

Turk. J. Phys., **22**, (1998), 505-510.
Full text: pdf
Other articles published in the same issue: Turk. J. Phys.,vol.22,iss.6.