

Physical Properties of Pd-Al Binary Metal Alloys Investigated by Using Molecular Dynamics Simulation Methods

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Abstract

In this study, some statical and dynamical properties of transition metals and metal alloys are investigated by using molecular dynamics simulation method and Quantum Sutton-Chen (Q-SC) inter atomic potential. The simulation is specified for Pd, Al transition metals and Pd-Al binary metal alloys in the liquid form for different concentrations and at various temperatures. Statical properties such as Pair Distribution Function, $g(\mathbf{r})$, Structure Factor, $S(\mathbf{q})$ and dynamical properties such as Einstein Relations, Intermediate Scattering function, $F(\mathbf{q}, \mathbf{t})$ and Dynamical Structure Factor, $S(\mathbf{q}, \omega)$ are calculated for various values of wave vector \mathbf{k} .

Keywords : Pair Distribution function $g(\mathbf{r})$, Structure Factor $S(\mathbf{q})$, Intermediate Scattering Function $F(\mathbf{q}, \mathbf{t})$, Dynamic Structure Factor $S(\mathbf{q}, \omega)$.

References

1. Yoshitaka Kimura, Yue Qi, T. Çağın, and William A. Goddard, Phys.Rev.B, 59, 5 (1999-1)
2. Finnis, M. Materials World, 9, 12, (2001)
3. H.Rafii Tabar and A.P. Sutton, Phil.Mag.Lett. 63, 217 (1991)
4. Waseda, Y. "The Structure of Non Crystalline Materials" McGraw-Hill Inc. 1980
- 5 McQuarrie, D. A. "Statistical Mechanics" Harper and Row, New York (1976) [Chp. 2]
6. Heyes, M. D. "The Liquid State" John Willey and Sons. Sussex 1998
7. Tildesley, D. J. "Computer Simulation of Physics", Clarendon Press - Oxford 1987
8. Canales, M. Padro, J. A. Physical Review E, 56,2 (1997)
9. Rahman, A. Phys. Rev. Lett., 32,52 (1972a)