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Extraction of an effective pair potential from a many body potential of metallic systems XUEYU SONG, TOMAZ URBIC, VADIM WARSHAVSKY, CAI-ZHUANG WANG, Department of Chemistry and Ames Laboratory, Iowa State University, Ames, IA 50011 — For metallic systems most reliable descriptions are given by many body potentials and on the other hand most of successful liquid theories are formulated based upon pair potentials. The effective state-dependent pair intermolecular potential can be calculated as a solution of the modified hypernetted chain (MHNC) integral equation. With an initial guess of the bridge function in this equation either from the conventional MHNC approximation [1] or from the Fundamental Measure Density Functional Theory [2] several iterations with simulations lead to converged pair potential [3]. In this report we use the both methods to extract an effective pair potential from an embedded atom model potential of aluminum and a tight-binding many-body potential of silicon [4]. Using the effective pair potential the calculated phase diagrams agrees well with the phase diagram from direct simulations via the original many body potential. 1. Y.Rosenfeld and N.W.Ashcroft, Phys.Rev.A 20, 1208(1979). 2. Y.Rosenfeld and G.Kahl, J.Phys.:Condens.Matter 9, L89(1997). 3. L.Reatto, D.Levesque and J.J.Weis, Phys.Rev.A, 33, 3451(1986). 4. C.Z.Wang, B.C.Pan, and K.M.Ho, J. Phys. : Condens. Matter 11, 2043 (1999).

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