Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Solid to liquid transition and the potential energy surface of sodium clusters IGNACIO L. GARZON, Instituto de Fisica, Universidad Nacional Autonoma de Mexico, JUAN A. REYES-NAVA, LUIS A. PEREZ — Thermal stability properties, the melting-like transition, and heat capacities of Na_n, n=13-309, clusters have been investigated using a many-body potential energy surface and molecular dynamics simulations. The characteristics of the solid-liquid transition in the sodium clusters are analyzed by calculating physical quantities like caloric curves, heat capacities, and root-mean-square bond length fluctuations using simulation times of several nanoseconds. Distinct melting mechanism are obtained for the sodium clusters in the size range investigated. The calculated melting temperatures show an irregular variation with the cluster size, in qualitative agreement with recent experimental results. By performing a survey of the cluster potential energy landscape, it is found that the width of the distribution function of the kinetic energy and the spread of the distribution of the potential energy minima (isomers), are useful features to determine the different behavior of the heat capacity of the function of the cluster size. Density functional calculations were performed to test the accuracy of the many-body potential energy surface to model the bonding existing in sodium clusters. Acknowledgments: This work was supported by CONACyT No. 43414-F, UNAM-DGAPA No. IN4402, and DGSCA UNAM Supercomputing Center.

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Date submitted: 30 Nov 2004 Electronic form version 1.4