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Theory of the Melting of Confined Nanocrystals DARYL CHRZAN, Q. XU, I.D. SHARP, Materials Science and Engineering, University of California, Berkeley and Materials Sciences Division, Lawrence Berkeley National Laboratory, D.O. YI, Applied Science and Technology, University of California, Berkeley, C.W. YUAN, C.Y. LIAO, A.M. GLAESER, Materials Science and Engineering, University of California, Berkeley and Materials Sciences Division, Lawrence Berkeley National Laboratory, J.W. AGER III, Materials Sciences Division, Lawrence Berkeley National Laboratory, E.E. HALLER, Materials Science and Engineering, University of California, Berkeley and Materials Sciences Division, Lawrence Berkeley National Laboratory — Recent measurements of the melting point of Ge nanocrystals embedded within a silica matrix reveal that the nanocrystals can be heated approximately 200 K above the bulk melting point before melting, and cooled approximately 200 K below the bulk melting point before solidification. This behavior is in marked contrast to that observed for free standing nanocrystals. We have developed a classical, continuum thermodynamic model which demonstrates that the phenomenon is caused by kinetic barriers to the nucleation of the liquid phase. The kinetic barriers are associated with the density increase upon melting of Ge and the fact that liquid Ge does not wet silica. The model provides a quantitative description of the experimental observations. This research is supported by the U. S. Department of Energy under contract No. DE-AC02-05CH11231.

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