Nucleation of Monovalent Metal Particles from Metastable Vapor

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Molecular beam studies demonstrate that molten clusters of alkali metals (Li, Na, K, Rb, Cs, and Fr) and coinage metals (Cu, Ag, and Au) have pronounced quantum confinement effects resulting in particularly stable clusters with 2, 8, 18-20, 34, 40, … atoms.[1] These clusters are called magic numbered clusters. Due to their relative stability, the magic numbered clusters are more prevalent in a supersaturated vapor than a classical model would suggest. Therefore they may promote cluster growth, as opposed to monomer growth, during nucleation from supersaturated vapor.

We present a model for calculating nucleation rates for the condensation of monovalent metal vapors. A Jellium model [2] is used to estimate cluster properties. Cluster growth is permitted by numerically solving the coupled master equations for the stationary state cluster concentrations. The model suggests that the effects of cluster stability and growth mechanism are non-linear and strongly coupled. Rates calculated using the improved model differ by several orders of magnitude relative to the classical nucleation rate theory. Onset conditions and calculated rates compare favorably with experimental data for alkali and coinage metals where available. Verifiable predictions are made for the other metal vapors. Details of the methods and results are given in Ref. [3]. Opportunities for extension of the model to metals with higher and/or multiple valences are to be discussed during the oral presentation of this work.

[1] H. Haberland, (ed.) Clusters of Atoms and Molecules, (Springer-Verlag, New York, 1984).
[2] M. Y. Chou and M. L. Cohen, Electronic shell structure in simple metal clusters, *Phys Lett. A* **113**, 420 (1986).
[3] R. Bahadur and R. B. McClurg, Nucleation Rate for the Condensation of Monovalent Metals, *J. Chem. Phys.*, In Press (2004).