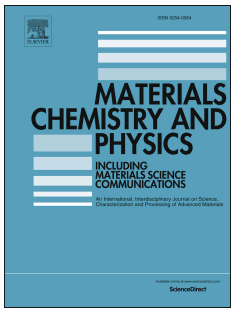
Accepted Manuscript



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PII: S0254-0584(17)30075-5

DOI: 10.1016/j.matchemphys.2017.01.049

Reference: MAC 19456

To appear in: *Materials Chemistry and Physics*

Received Date: 11 July 2016

Revised Date: 9 October 2016

Accepted Date: 14 January 2017

Please cite this article as: J. Zhu, Q. Fu, Y. Xue, Z. Cui, Accurate thermodynamic relations of the melting temperature of nanocrystals with different shapes and pure theoretical calculation, *Materials Chemistry and Physics* (2017), doi: 10.1016/j.matchemphys.2017.01.049.

Accurate thermodynamic relations of the melting temperature of nanocrystals with different shapes and pure theoretical calculation

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ABSTRACT

Based on the surface pre-melting model, accurate thermodynamic relations of the melting temperature of nanocrystals with different shapes (tetrahedron, cube, octahedron, dodecahedron, icosahedron, nanowire) were derived. The theoretically calculated melting temperatures are in relative good agreements with experimental, molecular dynamic simulation and other theoretical results for nanometer Au, Ag, Al, In and Pb. It is found that the particle size and shape have notable effects on the melting temperature of nanocrystals, and the smaller the particle size, the greater the effect of shape. Furthermore, at the same equivalent radius, the more the shape deviates from sphere, the lower the melting temperature is. The value of melting temperature depression of cylindrical nanowire is just half of that of spherical nanoparticle with an identical radius. The theoretical relations enable one to quantitatively describe the influence regularities of size and shape on the melting temperature and to provide an effective way to predict and interpret the melting temperature of nanocrystals with different sizes and shapes.

1. Introduction

The melting temperature of nanocrystals presents considerable depression compared with their bulk counterparts due to the large surface-to-volume ratio of nanocrystals [1-6]. The melting process is often involved in the preparations, studies and applications of nanocrystals, and the correlative research on melting has always been one of the hotspots in the academic field. Early in 1909, Pawlow proposed a