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Prediction of Melting Temperature of Nanoclusters by Atomistic Simulations

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The calculation of the melting temperature of materials is of fundamental interest, representing a fundamental understanding of the equilibrium properties of system The melting line may be determined if we know the Gibbs free energy of both solid and liquid phases as a function of temperature and pressure The difficulty in the application of this simple thermodynamic principle to nanocluster is that the free energy of the system cannot be trivially calculated On the other hand, in conventional molecular dynamics simulations, the melting temperature of nanoclusters can be estimated from the caloric curve directly by measuring the total potential energy of system with the slow increase of temperature However, due to the limitation of simulation time scale in molecular dynamics, this method does not guarantee thermodynamics equilibrium in spite of granting that the superheating of solid cluster is negligibly small Therefore, we introduce an alternative way of determining the melting temperature using umbrella-sampling method combined with constrained molecular dynamics simulation. In this method, we can obtain the Landau free energy curves near the estimated melting temperatures and determine the melting point by interpolating the relative free energy difference between the solid and liquid phases In this research, the melting point of 459-atom Au nanocluster was predicted based on the semi-empirical embedded-atom method Additionally, the particular melting behavior of Au nanoclusters reported by molecular dynamics simulations [Phys. Rev Lett 81, 2036 (1998)] could be explained well by the calculated free energy curve.

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SiO_2 및 TiO_2 첨가가 PMN-35PT의 미세조직에 미치는 영향

Effect of SiO_2 and TiO_2 addition on the Microstructure Evolution in PMN-35PT System

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PMN-35PT 단결정의 우수한 압전 물성이 보고 되면서 양질의 단결정을 제조하기 위한 많은 연구가 이루어졌다 특히 최근에는 높은 제조 단가를 낮추려는 시도로 고상 단결정 성장법을 통한 단결정 제조 노력이 활발히 이루어지고 있는데, 이 경우 미세조직의 효과적인 제어가 필수적이다 그래서 PMN-35PT 세라믹스의 미세조직 변화에 있어 자연계에 가장 흔히 존재하는 SiO_2와 복잡한 분말 준비 과정에서 미반응 물질로 개재될 수 있는 TiO_2가 미치는 영향을 연구하였다 SiO_2의 첨가는 PMN-35PT 계의 쌍정 생성을 촉진하고, 결과적으로 쌍정을 가진 입자들만이 비정상적으로 성장하는 결과(TPRE)를 보인 반면, TiO_2의 첨가는 {001}면이 잘 발달된 입방정 형태의 비정상 입자를 유도하였다 본 연구에서는 TiO_2에 의한 비정상 입성장의 생성 기구를 저각 입계에 의한 핵생성 촉진(GBRE) 효과로 설명하였다