Crystallization of Aluminum droplet at low supercooling: theoretical analysis by homogeneous nucleation model

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Crystallization in an undercooled Aluminum (Al) droplet occurs via the formation of crystalline nuclei by homogeneous or heterogeneous nucleation and successive growth of nuclei. Clusters of a new phase appear in the system due to fluctuations and after reaching of a critical size i^*, nuclei form a new phase. Crystallization event at low undercooling 6.4 ^oC of 9.91 mg of a compact Al sample was detected using isothermal differential scanning calorimetry (DSC) after several tenths of minutes. Standard analysis based on Johnson-Mehl-Avram-Kolmogorov (JMAK) model is not appropriate in this case [1] as Avrami parameter n, which is closely connected to the dimensionality of the system, is too low to fit the crystallization data via JMAK model. Al growth rate is extremely high [2] and that is why we presume that the time delay of crystallization, detected by DSC, is slightly higher then nucleation time delay. Homogeneous nucleation model is applied to determine the basic characteristics of nucleation: the size distribution of nuclei, nucleation rate, total number of nuclei and crystallization fraction at the nucleation process. Interfacial energy σ was selected to get only several supercritical nuclei within the Al droplet and the kinetic barrier of nucleation, E, was chosen to get a reasonable value in the time delay of nucleation due to high Al growth rate. The number of atoms in a liquid Aluminum droplet decreases with time as a formation of a new crystalline phase occurs. In consequence, the decrease in stationary nucleation occurs. It is shown that the decrease in the number of atoms in a liquid Al droplet is predominantly caused by a formation of subcritical clusters.

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[1] Z. Kožíšek, R. Král, P. Zemenová, *Homogeneous nucleation and crystallization model of Aluminum droplet based on isothermal DSC analysis*, accepted to J. Therm. Anal. Calorim. https://doi.org/10.1007/s10973-022-11497-z.

[2] G. Sun, J. Xu, P. Harrowell, *The mechanism of the ultrafast crystal growth of pure metals from their melts*, Nature Mater. 2018 (17) 881887. https://doi.org/10.1038/s41563-018-0174-6.