Time-Resolved Powder Diffraction Study of the Melting of Palladium Nanocrystals

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Workshop on Ultrafast X-ray Techniques for Monitoring Dynamic Structural and Electronic Responses at the Nanoscale, APS Users Meeting, May 2021

Melting of simple metallic nanoparticles is widely believed to be nucleated at the surface, where lower-coordination sites are available. This has been seen in gold nanoparticles using XFEL techniques [1]. Vibrations are expected to be larger at surfaces, so the Lindemann criterion can be reached at lower temperatures there. Facetted nanoparticles have edge sites and vertices where the coordination is even lower than at flat surfaces. It has been known since the 1970's that the melting point of gold nanoparticles is reduced all the way down to room temperature at sufficiently small particle sizes [2]. Optical pump – X-ray probe experiments, as performed at 7-ID, offer a good possibility to observe ultrafast melting with a laser in order to visualize the location of the nucleation event and the progression of melting. The expected timescale can be estimated to be in the nanosecond range from classical thermal diffusion calculations which establish the concept of a melt-front traveling at sub-sonic velocity [3]. We report here on our first attempts to use X-ray powder diffraction with Pair-Distribution Function analysis at 7-ID to look at reversible melting phenomena in palladium nanoparticles.

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[2] Size effect on the melting temperature of gold particles, P. Buffat and J-P. Borel, Phys. Rev. A **13** 2287 (1976)

[3] Melt-front Dynamics in Polycrystalline Gold Thin Films Tadesse A. Assefa, Yue Cao, Soham Banerjee, Sungwon Kim, Dongjin Kim, Sunam Kim, Jae Hyuk Lee, Sang-Youn Park, Intae Eom, Jaeku Park, Daewoog Nam, Sangsoo Kim, Sae Hwan Chun, Hyojung Hyun, Kyung Sook Kim, Pavol Juhas, Emil S. Bozin, Ming Lu, Changyong Song, Hyunjung Kim, Simon J. L. Billinge and Ian K. Robinson, Science Advances **6** eaax2445 (2020)