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Determination of Melting and Surface Premelting Points of Silver Nanoparticles by Molecular Dynamics Simulation H. Alarifi\* <a href="mailto:halarifi@uwaterloo.ca">h. Alarifi\*</a> <a href="halarifi@uwaterloo.ca">h. Alarifi\*</a> <a href="halarifi@uwaterloo.ca">h. Alarifi\*</a> <a href="halarifi@uwaterloo.ca">h. Alarifi\*</a> <a href="halarifi@uwaterloo.ca">h. Alarifi@uwaterloo.ca</a>, Department of Mechanical and Mechatronics Engineering, Centre for Advanced Material Joining, University of Waterloo, 200 University Ave. W, Waterloo, ON N2L 3G1; M. Atis <a href="halarifi@uwaterloo.ca">h. Alarifi@uwaterloo.ca</a>, Department of Material Joining, University of Waterloo, 200 University Ave. W, Waterloo, ON N2L 3G1; M. Atis <a href="halarifi@uwaterloo.ca">h. Alarifi@uwaterloo.ca</a>, Department of Material Joining, University of Waterloo, 200 University, Polyment of Physics, Nevsehir University, 2000 Evler, 50300 Nevsehir, Turkey; C. Ozdogan <a href="halarifi@uwaterloo.ca">h. Alarifi@uwaterloo.ca</a>, A. Hu

A molecular dynamics (MD) simulation based on the embedded atom method (EAM) was conducted on different sizes of Ag nanoparticles (NPs) with diameters of 4 nm to 20 nm to find melting and surface premelting points. A comparison between our simulation and other theoretical models for melting was reported. Obtained melting point values of the NPs showed good agreement with Hanszen's model for 8 nm and larger particles and good agreement with the liquid drop model and Shi's model for smaller particles. Melting of Ag NPs of 8 nm and larger diameters started by forming quasi-liquid lakes on the surface that grew and coalesced to form a liquid layer of 2 nm thickness, which is about 10 atomic layers. The liquid layer was then expanded to the solid core as the temperature increased to the melting point of the NP. The ratio of the liquid shell thickness to the NP radius shows a linear relationship with temperature. Ag NPs with a diameter smaller than 8 nm melted homogenously without passing through surface premelting stage.

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