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A Molecular Dynamics Simulation of Platinum Nanoparticle Formation During Vapour Deposition

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Abstract content
   (Max 300 words)

As modern concerns about carbon emissions increase the desire for platinum nanoparticles to be used as a catalyst in the catalytic converters of cars also increases. Therefore it is important to understand how platinum nanoparticles form in order to manufacture the desire nanoparticles with the correct size and shape. A unique insight regarding the different parameters and process can be gained by using Molecular Dynamics (MD) to simulate the formation of the platinum nanoparticles. For the simulations in this study, the Sutton-Chen potential was used since it is well suited for simulating FCC metals such as Pt [1]. This study focused on the growth of Pt nanoparticles during physical vapour deposition. In the model used, Pt atoms are projected from random locations above a surface towards the surface. This simulation was done for different evaporation rates and temperatures in order to investigate their effect on the growth of the nanoparticles. When varying the surface temperatures it was found that the structures at higher temperatures are more closely packed compared to that at lower temperatures. By lowering the evaporation rate the atoms have more time for movement at lower temperatures to form closed structures. It was also noticed that the structures tend to be single layer structures on the surface. This can be explained by looking at the energies required to move the atoms between different positions on the structures and the minimisation of the energies at those positions.
[1] Long-range Finnis–Sinclair potentials, A. P. Sutton, J. Chen, Philosophical Magazine Letters, Vol. 61, Iss. 3, 1990

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JJ Terblans,Department of Physics, University of the Free State, Email: terblansjj@ufs.ac.za

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Primary author: Mr WESSELS, Leon (UFS)

Co-authors: Prof. SWART, Hendrik (UFS); Prof. TERBLANS, Koos (UFS)

Presenter: Mr WESSELS, Leon (UFS)

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