Monte Carlo Simulations of Helium and Neon Ions Beam Induced Deposition

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The new Gas Field Ion Microscope is able to deposit and etch material at the nanoscale in a highly controlled manner, but in order to exploit this capability it is necessary to have a detailed quantitative model of the process. A Monte Carlo simulation for He+ and Ne+ ion beam induced deposition (and etching) has been developed which provides data in excellent agreement with the observed experimental results over a wide range of experimental conditions. The ion beam induced nanoscale synthesis of PtC_x (where x~5) using the trimethyl (methylcyclopentadienyl)platinum(IV) ($MeCpPt^{IV}Me_3$) precursor is investigated by performing Monte Carlo simulations of helium and neon ions integrated with a gas handling routine to mimic the precursor adsorption and decomposition.

The simulation results show that the helium beam leads to more lateral growth relative to the neon beam because of its larger interaction volume. Figure 1 depicts resting positions of 10,000 ions for both helium and neon simulations. It shows that much energy is dissipated in smaller volume for Ne ions as compared to that of helium ions. The lateral growth of the nanopillars is dominated by molecules deposited via secondary electrons in the both simulations. Notably, the helium pillars are dominated by SE-I electrons whereas the neon pillars by SE-II electrons as shown in Figures 2 and 3 respectively.

Using a low precursor residence time of 70μs resulting in an equilibrium coverage of ~ 4%, the neon simulation has a lower deposition efficiency (3.5%) compared to that of the helium simulation (6.5%). At larger residence time (10ms) and consequently larger equilibrium coverage (85%) the deposition efficiencies of helium and neon increased to 49% and 21%, respectively; which is dominated by increased lateral growth rates leading to broader pillars. The nanoscale growth is further studied by varying the ion beam diameter at 10 ms precursor residence time. The study shows that total SE yield decreases with increasing beam diameters for the both ion types. However, the helium has the larger SE yield as compared to that of neon in the both low and high precursor residence time, and thus pillars are wider in all the simulations studied.
Finally, experimentally we have shown that He ion deposited material has a larger room temperature resistivity (~3.5×10^4 - 2.2×10^5 μΩ-cm) and temperature dependent transport behavior consistent with a granular material in the weak

intergranular tunnel coupling regime. Conversely Ne ion deposited material has a much lower room temperature resistivity (~600 – $3.0x10^3$ μΩ-cm) and temperature dependent electrical behavior representative of strong intergranular coupling. The Ne ion deposited nanostructure has larger platinum nanoclusters, which is rationalized via Monte-Carlo ion-solid simulations that show the neon energy density deposited during growth is much larger due to the smaller ion range as shown in Figure 4. The plots depict the nuclear energy deposited via Helium and Neon simulations respectively. The observed platinum grain coarsening and subsequently lower resistivity for the Ne ions beam induced deposits is correlated to the enhanced platinum mobility via the enhanced nuclear stopping of the Neon ions.

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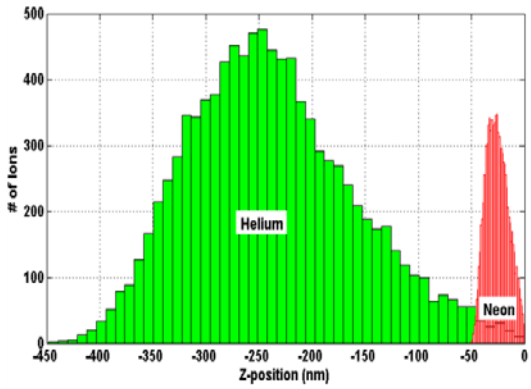

Figure 1: Histogram of resting position of Helium ions (green) and neon ions (red) in z-direction.

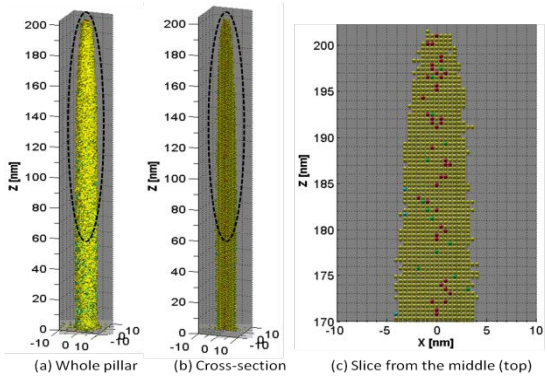

Figure 2: Deposited nanostructures of PtC_5 via Helium ion simulation at 70 μs precursor residence time.

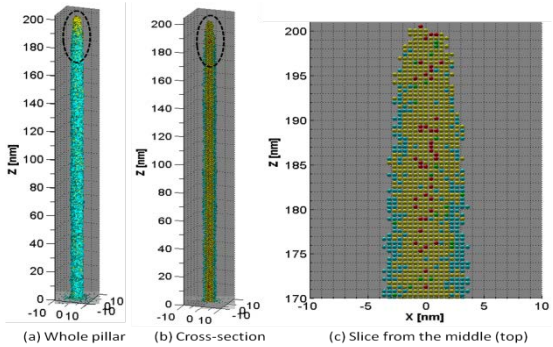

Figure 3: Deposited nanostructures of PtC_5 via Neon ion simulation at 70 µs precursor residence time.

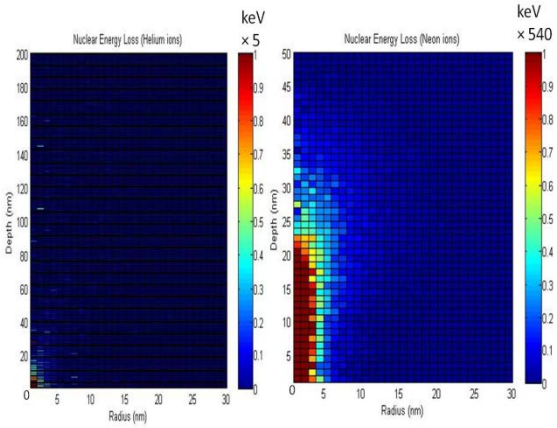

Figure 4: Radially averaged nuclear energy dissipated via Helium (left) and Neon (right) ions simulation (10,000 ions).