Supplementary material: Effects of core electrons on stopping power in hellium-irradiated aluminum nanosheet

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In this supplementary material, we present the stopping power curve calculated using simulation cell sizes of $2 \times 2 \times 2$, $3 \times 3 \times 3$ and $4 \times 4 \times 4$ and the ratio of kinetic energy of target atom (E_{KT}) to kinetic energy of projectile (E_{KP}) during collision under channeling and off-channeling condition.

A. The impact of simulation cell size

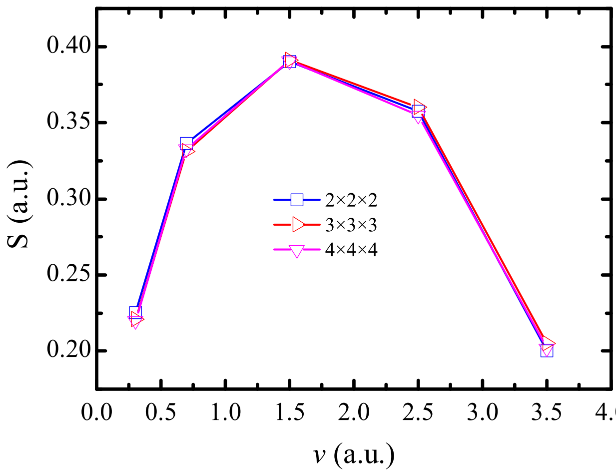

FIG. 1. The stopping power curve calculated using simulation cell sizes of $2 \times 2 \times 2$, $3 \times 3 \times 3$ and $4 \times 4 \times 4$. The valence electrons configurations of Al pseudopotential is $3s^2 3p^1$. For all simulations, the projectile is incident along the channeling trajectory.

The structure of Al film we investigated is $2 \times 2 \times 2$ supercell, consisting of 32 Al atoms. This simulation was compared to a larger simulation cell with 108 Al atoms ($3 \times 3 \times 3$) and 256 Al atoms ($4 \times 4 \times 4$). The cubic lattice parameter is 4.039 Å.

Fig. 1 shows the stopping power curves calculated using different size simulation cell of $2 \times 2 \times 2$, $3 \times 3 \times 3$ and $4 \times 4 \times 4$. The results show that no appreciable finite size errors were found. The supercell size is chosen to meet the computational requirements of cost control while minimizing the impact of grain size on the research.

B. The role of nuclear stopping

Fig. 2 shows the ratio of kinetic energy of target atom (E_{KT}) to the kinetic energy lost by the projectile (ΔE_{KP}) during collision under channeling condition. Fig. 3 shows that the Ratio of kinetic energy of target atom (E_{KT}) to the kinetic energy lost by the projectile (ΔE_{KP}) during collision under off-channeling condition. In the velocity range of our study, when the velocity is 0.1 a.u., the ratio can reach 2.6 % at the highest. As the velocity increases, the ratio decreases rapidly. For off-channeling trajectories, the ratio of the E_{KT} to the ΔE_{KP} is given. When the projectile is very close to the target atom, the ratio increases. But during the whole collision process, the target kinetic energy is very small.

The nuclear motion is allowed in our simulation, including the nuclear stopping effect. However, the kinetic energy of the target atom during the whole collision process is so small that the S_n is negligible.

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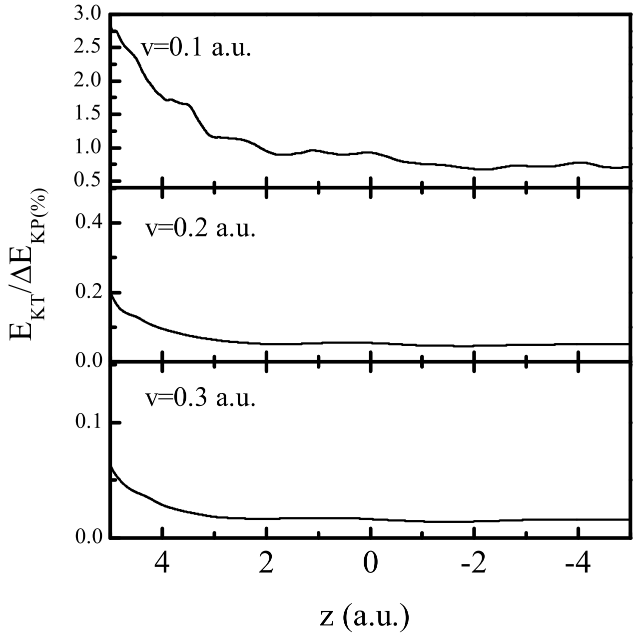

FIG. 2. Ratio of the kinetic energy of the target atom (E_{KT}) to the kinetic energy lost by the projectile (ΔE_{KP}) during collision as a function of the projectile position for channeling trajectory.

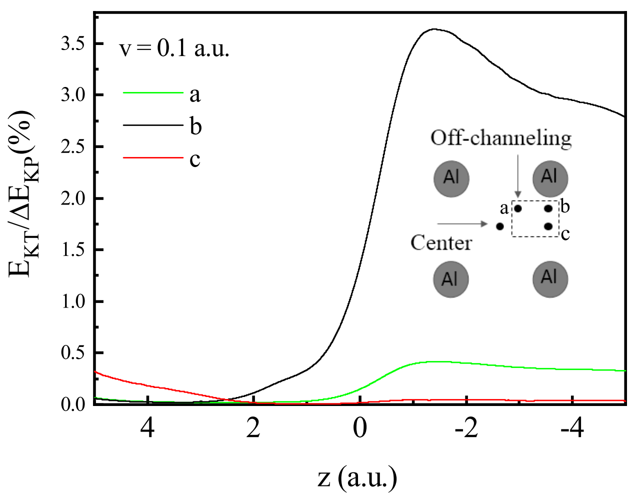

FIG. 3. Ratio of the kinetic energy of the target atom (E_{KT}) to the kinetic energy lost by the projectile (ΔE_{KP}) during collision as a function of the projectile position for off-channeling trajectory.