EFFECTS OF AlN IRRADIATION WITH SWIFT HEAVY IONS: MULTISCALE MODELLING

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This work focuses on modeling the radiation effects of swift heavy ions (SHI, SHI, $m > 4m_p, E > 0.5\frac{MeV}{nucl}$) in AlN. This material was chosen because it holds promise for use in nuclear reactors as an inert matrix for fuel [1]. The development of such a matrix is important, as humanity needs to find ways to utilize plutonium and other minor actinides.

As is well known, all processes occurring within the track of a swift heavy ion can be well-separated in time [2], which enables the use of multiscale modeling. To describe the ion's impact and subsequent electron kinetics, the TREKIS model, based on Monte Carlo methods [2], was used. Following this, molecular dynamics (MD) methods [3] were applied during the atomic dynamics stage to trace the movement of atoms. The irradiating ions used were Ar, Xe, and Bi, with energies of 100, 158, and 700 MeV, respectively.

The first step involved modeling the ion impact on the material and the subsequent electron kinetics of AlN with the help of the TREKIS model. The method is based on the dynamical structure factor and the complex dielectric function formalism. In this framework, the scattering cross-section is calculated with applying the energy loss function $\mathbf{Im}\left[\frac{-1}{\boldsymbol{\varepsilon(\omega,q)}}\right]$, that can be reconstructed from experimental or calculated data – complex refractive index of the material and x-ray photon attenuation length, where $\boldsymbol{\varepsilon(\omega, q)}$ is complex dielectric function of the material [2].

After calculating the loss function, Monte Carlo modeling of the ion impact on the material and subsequent electron kinetics of AlN were performed. As shown in Figure 1a, by 100 femtoseconds after the ion impact, the energy transferred to the electron subsystem dissipates, and regions with a constant electron density emerge. Figure 1b illustrates that the decrease in mass and energy of the swift heavy projectile leads to a reduction in the energy transferred to the ion subsystem.

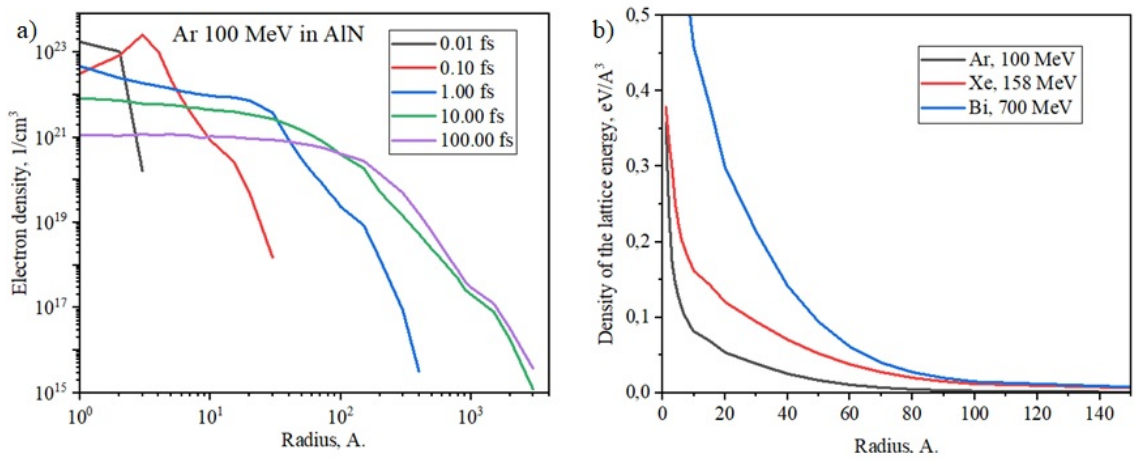

Fig. 1. a) radial dependence of the electron density in ion track, b) density of the energy transferred into AlN lattice (100 fs after ion impact)

The next step of the study involved modeling the relaxation of the ionic subsystem using molecular dynamics, both in the bulk and at the surface. To do this, it was first necessary to define an interatomic potential that best describes the interatomic forces. In this work, the Tersoff potential [4] and the Vashishta potential [5] were compared. To evaluate their accuracy, the elastic constants, cohesive energy, and lattice parameters at temperatures of 0 and 300 K were calculated using both potentials. Additionally, as an important test, the melting temperature of AlN was calculated. It was found that the rapid increase in atomic displacement, indicating the melting of the material, occurs entirely in the boundary region, which aligns with the experimentally defined melting temperature range of the material when the Vashishta potential is applied. Therefore, the Vashishta potential was selected for use in future modeling.

The first part of the study focused on modeling the irradiation effects in bulk samples. The results are shown in Figure 2. As seen in the images, no track formation occurs after Ar ion impact and nanometer-sized defect clusters form after Xe and Bi ion irradiation. The recovery time of the damaged region after Bi ion impact is approximately 30 ps.

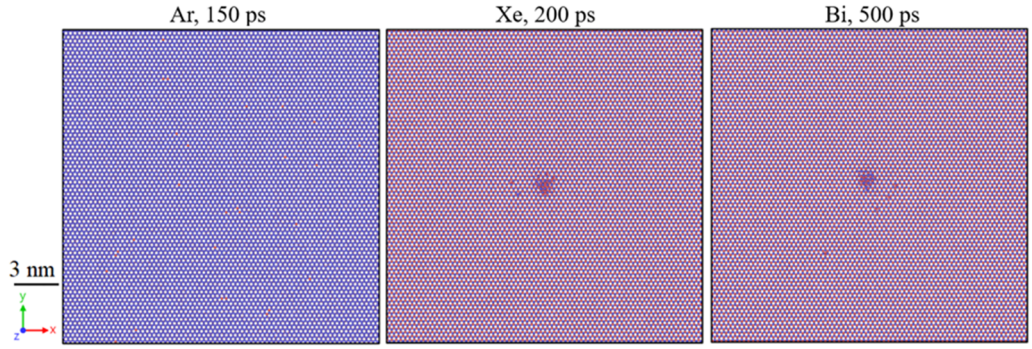

Fig. 2. AlN atoms positions after the ions impact (bulk model). Energies of ions: Ar – 100 MeV, Xe - 158 MeV, Bi – 700 MeV

The second part of the study involved modeling the surface effects caused by SHI irradiation. The results are presented in Figures 3 and 4. As seen, Ar ions do not create any significant damage on the surface or in the near-surface region, while Xe ions create a surface hillock with a height of about 1.5 nm and a conical near-surface latent track. The difference in behavior can be attributed to the fact that after Xe irradiation, the sample reaches its melting temperature, unlike with Ar ions, causing atoms to be expelled from the damaged region. The most pronounced damage occurs with the Bi ion impact – it creates a hillock with a height of approximately 8 nm and cavities in the near-surface region. The formation of the hillock is due to the strong protrusion of molten material from the damaged volume, resulting from significant heating and a rapid increase in pressure.

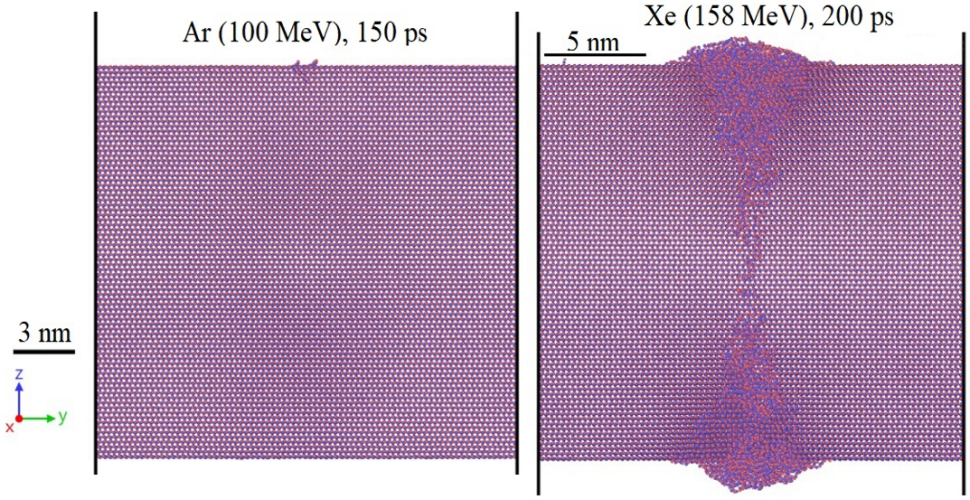

Fig. 3. AlN atoms positions after the Ar and Xe ions impact (open-surface model)

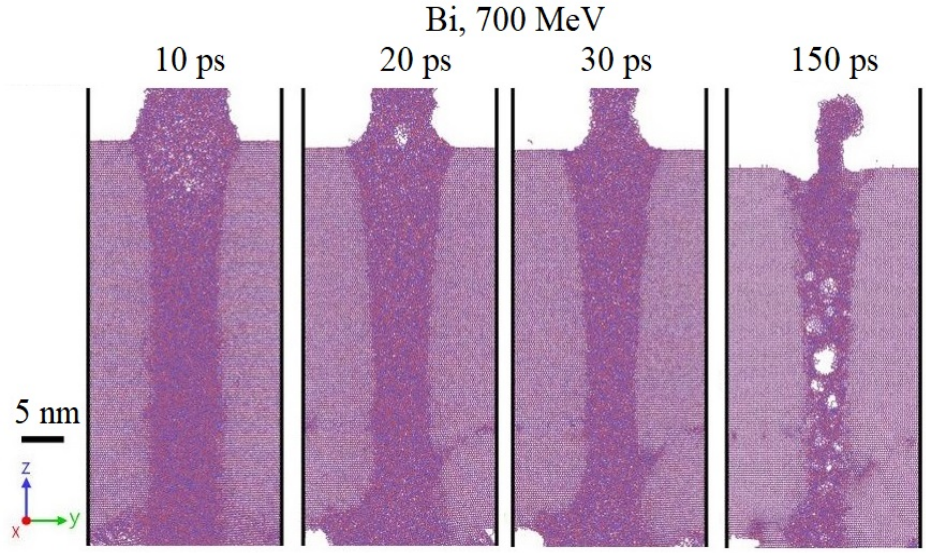

Fig. 4. AlN atoms positions after the Bi ion impact (open-surface model)

A conclusion can be drawn as follows:

a) In bulk AlN, ion tracks are not formed; only a few point defects along the ion trajectory are observed. This is due to the strong recrystallization ability of AlN.

b) Modeling of surface effects after Xe and Bi SHI impacts showed the formation of hillocks and cone-shaped tracks containing nanometer-sized cavities. This is because the presence of the surface suppresses the recrystallization processes.

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