ation effects of graphene need to be considered for design of graphene-based electronic devices. In addition, it was found that recrystallization of HOPG happens after swift heavy ion irradiation by using Raman spectroscopy. The results shown in Fig. 4 further evidence that the recrystallization can be randomly orientated. These fundamental researches indeed deepen the mechanistic understanding of ion-matter interactions.

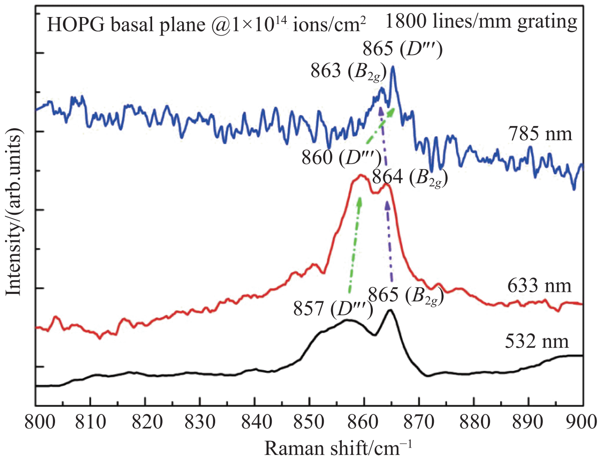

Fig. 4 (color online) The Raman spectra of the basal plane of the irradiated graphite with 40.5 MeV Sn ions using three different excitations.

4 - 16 Raman Investigation of Phonon Deformation in InP and GaN Induced by Swift Heavy Ions and Highly Charged Ions

Hu Peipei, Liu Jie, Zhang Shengxia, Zhai Pengfei, Zeng Jian, Duan Jinglai, Sun Youmei and Li Zongzhen

InP and GaN crystals were irradiated by swift heavy ions (SHI, ^{56}Fe and ^{209}Bi) with kinetic energies of 6.3 and 9.5 MeV/u and highly charged ions (HCI, 1.4 MeV $^{86}Kr^{12+}$ and $^{114}Xe^{20+}$). The irradiation effects induced by different types of irradiation were studied by Raman spectroscopy. Two new irradiation-induced vibrations observed at 294 and 338 cm^{-1} as shown in Fig. 1 are assigned to InP-like TO and LO first-order optical modes[1], respectively, and in Fig. 2 there observed additional optical modes at 291, 362 and 671 cm^{-1} in GaN[2] samples due to the irradiation of 352 MeV ^{56}Fe ions. In addition, we report for the first time the distance L between E_2(high) modes and $A1_1$(LO) modes decreased obviously with increasing ion fluences and electronic energy loss $(\mathrm{d}E/\mathrm{d}x)_\mathrm{e}$ in GaN samples after irradiated by Bi ions. In case of InP, the red-shift and strong asymmetrical broadening of the typical modes was detected after the irradiation. For HCI irradiation, in case of InP, the spectra shifted towards the lower wavenumbers with a maximum shift of 3.6 cm^{-1} induced by 1.4 MeV Kr^{12+} ion irradiation. The observed Raman shifts reveal the presence of lattice distortion induced by potential energy deposition in the samples. While in case of GaN, there is no change of the peak position.

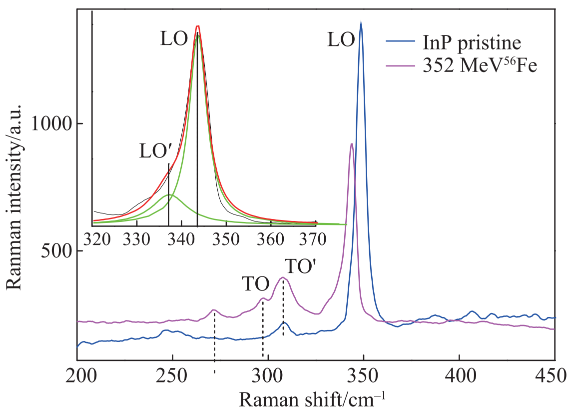

Fig. 1 (color online) Raman specra of InP before and after irradiation.

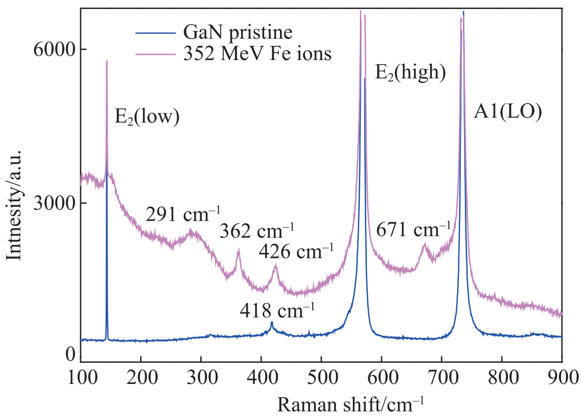

Fig. 2 (color online) Raman specra of GaN before and after irradiation.

The stress obtained from the Raman shift indicates that the lattice structure may be distorted around the defects and incorporated impurities due to SHI irradiation. The disorders induced in InP and GaN irradiated by SHIs were also investigated by TEM analysis and it was found that these results are consistent with Raman analyses. The residual stress observed in the Raman analyses is the consequence of defects induced in the samples after irradiation. Defects and disorders in the crystal break down the long-range order and translational symmetries and result in the modification of lattice vibrational modes of phonons. In our study we have considered only the first-order Raman scattering in pristine sample caused by the phonons with wave-vector k=0 (Γ point). However, because of the defects induced, the phonon modes that are contributing to the Raman scattering are not limited to those at the Γ point, but they are extended to the whole Brillouin zone in irradiated samples. This leads to the asymmetric broadening in phonon line-shape with a shift observed in the Raman spectra. Therefore the Raman peak shifts reflect the modification of lattice vibration mode, and can be regarded as a critical test of the stress induced in semiconductors irradiated by SHIs. The lattice stress resulting the Raman shift either belongs to the low wavenumber regime or high wavenumber regime depending on the tensile or compressive stress in the material.

References

[1] W. Pan, J. A. Steele, P. Wang, et al., Semiconductor Science and Technology, 30(9)(2015)094003.
[2] F. Moisy, M. Sall, C. Grygiel , et al., Nucl. Instr. and Meth. B, 381(2016)39.

4 - 17 Molecular Dynamics Simulation Studies of Crater Formation at the Surface of Gold Nanowire

Liu Wenqiang, Duan Jinglai, Cheng Yaxiong, Yao Huijun and Liu Jie

Previous works which studied the effects of cascade occurred at the metal surface indicate that, in case of most energy of the incident ion is deposited in the vicinity of the surface, the pronounced damage caused by viscous flow or by microexplosion can lead to creation of large number of adatoms and vacancy dislocation loops beneath the surface[1,2], or even formation of craters on the surface[3−6].

Bombardment with PKAs of kinetic energy higher than 10 keV will lead to the crater formation at the surface of nanowires. Fig. 1 shows one of the typical processes of the crater formation during the cascade induced by 20 keV PKA initiated at the surface. As can be seen in Fig. 1, in this particular case, that the crater was produced, the cascade core is relatively close to the surface. At the early stage of the cascade, high temperature and high pressure in the cascade core made the volume expanded rapidly and pushed the atoms outwards, which leads to cascade core intersecting with surface of the nanowire. At 3 ps, a void formation started and its volume is continued to expand with time. At 10.5 ps, the void reached its maximum size, at the same time the atoms started to retract, meanwhile the rim of the void started to rupture. During the retraction process, most of the atoms, which were expelled to the outside of the original surface, redeposited around the peripheries of the impinging point. And at the end, formation of a crater surrounded by adatoms was observed.

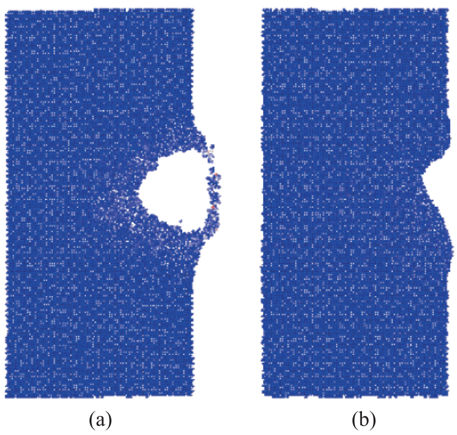

Fig. 1 (color online) Snapshots of the crater formation process in 13.8 nm gold nanowire induced by 20 keV PKA irradiation at the surface. (a) at 10.5 ps and (b) at 80.0 ps.

During the cascade evolution, most of the sputtered atoms were monomers and dimers. It was found that there were total 105 sputtered atoms, however, the crater consists of nearly 1 481 vacant sites. The result indicates that at most, the sputtering yield may contribute less than 10% to the crater's size. The crater was formed mainly due to three successive processes: (1) local melting of the materials in the cascade core under the high pressure inside; (2) further, it leads to some of the atoms, that originally located beneath several layers of the surface, were exploded to the outside; (3) re-deposition of most of these atoms in the surrounding of the impinging point. In this research, we recognize that the mechanism is very similar to the microexplosion produced by 20 keV self-bombardment at the surface of bulk Au. Formation of craters at the surface of nanowire or at the surface of bulk both show that there