Seminar

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Institute for Plasma Research

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Title: Low Energy Ion Beam Induced Modification of Functional Nanomaterials

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Time: 03:30 PM

Venue: Seminar Hall, IPR

Abstract

Low-energy ions are conventionally known to instigate an array of structural perturbations, including the generation of various defects and dislocations. A prominent example of such defects is the Frenkel defect, which manifests in crystalline solids as ion-induced collisions result in the creation of vacancies and the displacement of atoms into interstitial positions. With increased ion fluence, an accumulation of defects can lead to amorphization, while higher fluences can trigger recrystallization events due to augmented diffusion. Vacancies and interstitials, generated during this process, contribute to the development of internal stress within the nanostructure, eventually resulting in deformation and bending. Furthermore, low-energy ions yield significant sputtering effects, which can further alter the physical morphology and topography of the nanostructure. Beyond these physical alterations, it is noteworthy that low-energy ion beams can also induce chemical transformations on the surface. The presence of defects can introduce additional electronic states near the Fermi level in semiconducting oxides and transition metal dichalcogenides (TMDs), thereby altering their electrical conductivity. Additionally, vacancies can serve as traps for charge carriers and engender intriguing optical properties.

My initial emphasis is on elucidating the impacts of ion beam-induced modifications on 1D metal oxides and 2D TMDs. These modifications have resulted in homojunction formation at moderately higher ion energies in materials such as $SrMnO_3$ and WO_3. Interestingly, at lower ion energies, $SrMnO_3$ nanowires remain structurally unaltered, yet their surface undergoes a remarkable transition from superhydrophilic to superhydrophobic, indicative of surface chemistry alterations [1]. Conversely, low ion energies lead to the fragmentation of WO_3 nanorods due to surface modification and internal stress [2]. A detailed investigation was also carried out on heterojunction formation between $H_2Ti_3O_7$ and Cu_2O nanowires, which ensued from ion beam-induced surface defect formation and mixing [3]. A similar examination was conducted between WO_3 and $H_2Ti_3O_7$ nanotubes, revealing that $H_2Ti_3O_7$ serves to encapsulate WO_3, thus fortifying mechanical strength, preventing fragmentation, and enhancing conductivity. We scrutinized hydrogen gas adsorption in the core-shell heterostructure composed of WO_3 nanorods and $H_2Ti_3O_7$ nanotubes, achieving remarkable performance improvements following ion beam modification [4]. The potential benefits of ion beam modification for the gas adsorption properties of 2D transition metal dichalcogenide are exemplified by MoS_2. Remarkably, irradiated MoS_2 demonstrated superior ammonia sensing performance, attributable to the ion-induced creation of Mo vacancies [5]. Our elucidation of the structural modifications and junction formations induced by ion beams was supported by state-of-the-art TRI3DYN simulations. Furthermore, extensive employment of Density Functional Theory (DFT) simulations was integral in qualitatively describing the effects of ion beam-induced surface chemistry alterations, ultimately contributing to an improved understanding of the enhanced sensing capabilities of these modified systems.

References

1. **Manoj K. Rajbhar** et al. ***Applied Surface Science*** 2020, Volume 527, Pages 146683
2. **Manoj K. Rajbhar** et al. ***ACS Applied Nano Materials*** *2020, Volume 3, Pages 9064-9075*
3. **Manoj K. Rajbhar** et al. ***Applied Surface Science****, 2019, Volume 478, Pages 651-660*
4. **Manoj K. Rajbhar** et al. ***ACS Applied Nano Materials,*** *2023, Volume 6(1), Pages 212-227.*
5. **Manoj K. Rajbhar** et al. ***ACS Applied Nano Materials,*** *2023**,** Volume 6(1), Pages 5284-5297*