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RAINBOWS IN TRANSMISSION OF PROTON THROUGH THIN SILICON CARBIDE CRYSTAL

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Abstract. We propose the application of ion rainbows for the characterization of innovative functional materials. Thin silicon carbide (SiC) crystals exhibit highly promising qualities as a novel functional material, featuring unique physical and chemical properties suitable for applications in nanoelectronics, energy systems, and high-frequency, high-power devices. We aim to develop a theoretical framework for a novel materials characterization technique capable of visualizing crystalline structures. It will complement existing techniques in the field, offering a distinct advantage in directly characterizing both crystalline structure and composition.

1. INTRODUCTION

Characterization of crystals is an important part of materials science and engineering, crucial for understanding their structural, mechanical, electrical, and optical properties. By employing a variety of techniques, researchers unravel the intricate atomic arrangements and defects within crystalline materials, shedding light on their behavior and performance in various applications. From traditional methods like X-ray diffraction to cutting-edge approaches such as electron microscopy and atomic force microscopy, each characterization technique offers unique insights into the crystals' composition, orientation, and morphology. In this study, we introduce ion channeling through very thin crystals as a method for characterizing the crystallographic structure of materials. Ion channeling offers a unique approach to probe the structural properties of materials with high sensitivity and resolution. The ion channeling transmission characterization, based on the rainbow theory, presents a novel methodology specifically designed for analysis of the atomic arrangement and orientation within crystalline samples.

The ion channeling is an effect that occurs when a collimated ion beam is directed at a thin crystal oriented along a major crystallographic axis relative to the direction of the ion beam (see Gemmell 1974). In this phenomenon, ions traveling along specific crystallographic directions experience reduced scattering and can penetrate deeper into the crystal lattice, resulting in enhanced transmission through the material. This effect arises due to the alignment of the crystal lattice with the incident ion beam, allowing ions to travel through the open crystals' channels. If a crystal is sufficiently thin, ions will be transmitted through it and their scattering angles are subsequently detected, providing valuable information about the crystal's atomic structure and orientation. Additionally, in channeling, a significant effect occurs known as the crystal rainbow effect (see Petrović et al. 2000). This effect arises due to the singularity of the classical differential cross-section in particle scattering. It is characterized by strong focusing at a rainbow angle and an abrupt change in intensity/yield around it. Analysis shows that mathematically, the rainbows are singularities of the 2D mapping from the impact parameter (IP) plane to the scattering angle (SA) plane. Utilizing crystal rainbows, it is physically possible to describe the angular distribution of channeled ions in a way that rainbow lines represent it's "skeleton" (see Motapothula 2012), while this theory simplifies the characterization process by providing a comprehensive framework for analyzing ion channeling patterns (see Ćosić et al. 2019 and 2021, Hadžijojić et al. 2021 and 2023, Petrović et al. 2019, Starčević et al. 2021). In this work, we propose that the rainbow effect can be applied to the characterization of the SiC crystal.

2. RESULTS

The calculated rainbow patterns of channeled protons through thin Si, diamond, and SiC-3C crystals are presented. The method for their calculation is presented in Ref. (see Petrović et al. 2000). The thickness of all crystals was 24 nm, and the proton energy was 2 MeV. Si and C are cubic diamond-type monocrystals with a square crystal channel in the (001) orientation. The SiC polytype of interest in this work is SiC-3C, which forms a square channel in the (001) orientation. SiC-3C is a compound semiconductor characterized by rigid stoichiometry, where only a 50% Si and 50% C composition is allowed, meaning each Si atom has exactly four neighboring C atoms and vice versa. As already mentioned, the most prominent and intriguing aspect of the rainbow lines pattern is its representation as a "skeleton" of the ions' angular distribution. This indicates that all values of channeled ions' exit angles are constrained within rainbow lines, thereby defining the envelope of observable angular distributions.

Figs. 1(a) and (b) represent the rainbow lines in the IP and SA planes for the Si crystal, respectively, Figs. 1(c) and (d) depict the rainbow lines in the IP and SA for the diamond crystal, respectively, while Figs. 1(e) and (f) present the rainbow lines in the IP and SA planes for the SiC-3C crystal, respectively.

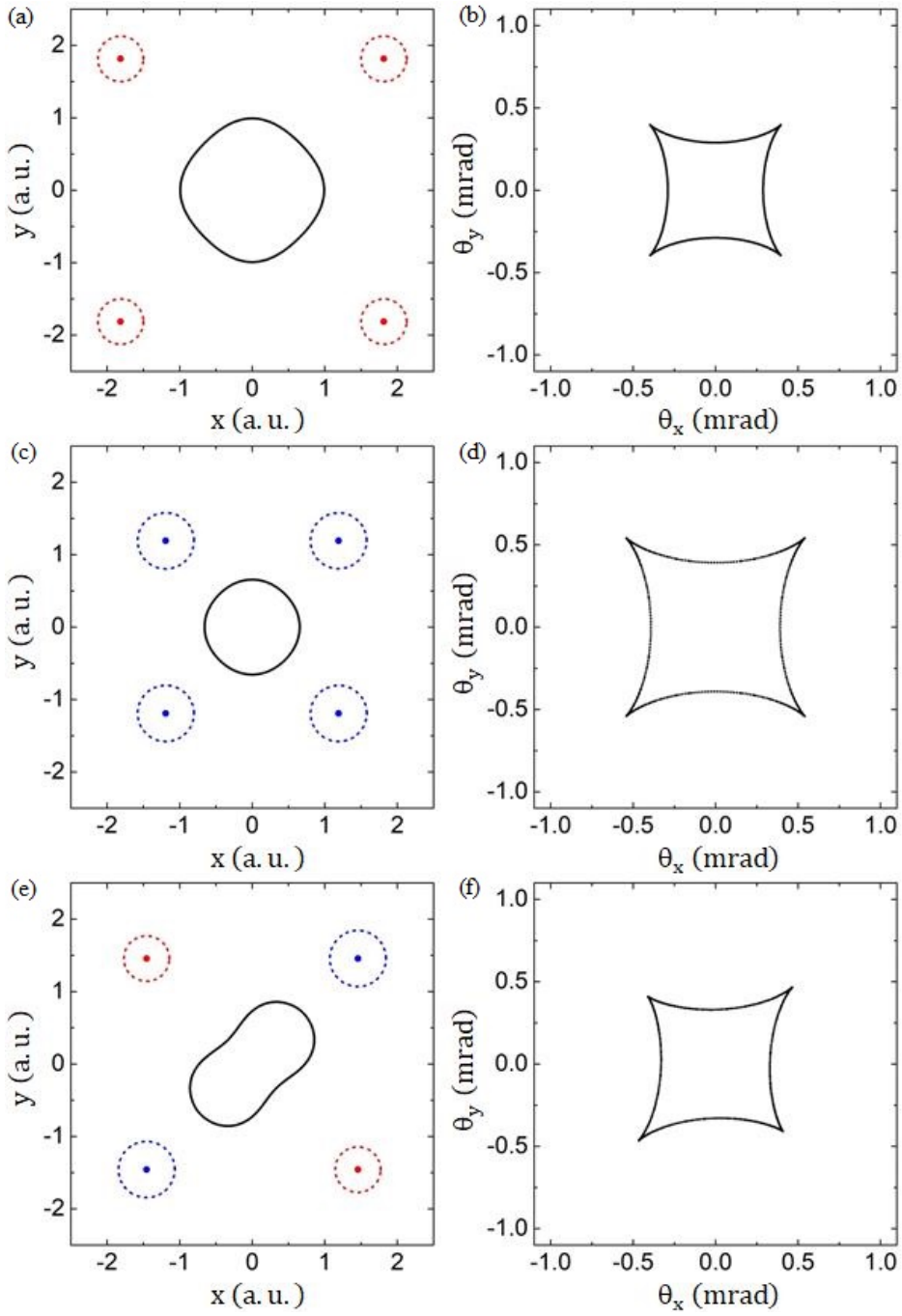

Figure 1: Rainbow lines in IP (left) and SA (right) plane for 2 MeV protons channeled through very thin Si (top), C (middle), and SiC (bottom) crystals.

For all crystals, the rainbow lines are designated by black color. For the Si crystal, in the IP plane, the positions of atomic strings forming the square channel

are shown as red dots, with red dotted circles indicating the Si atomic screening radius. In the SA plane, the rainbow line is in the shape of a square with cusped corners directed towards the atomic strings. For the diamond crystal, the blue dots indicate the positions of atomic strings defining the channel, while the blue dotted circles represent the C atomic screening radius. It is interesting to note that, as a consequence of a much smaller square channel of a diamond crystal in comparison with the Si one, the rainbow line for a diamond crystal is larger than for a Si crystal. This implies that the proton-diamond interaction in a square channel is effectively larger, although the proton-silicon atom interaction is larger than the proton-carbon atom interaction. Thus, we can conclude that the size of the rainbow line and the magnitude of its cusps vary for different crystals of the same thickness, allowing for the analysis and identification of crystal types using the crystal rainbow theory. As for the SiC-3C crystal, a deformed rainbow line occurs in the IP plane compared to the corresponding rainbow line for silicon and diamond crystals. Clearly, this is a result of the fact that the silicon repulses the rainbow line more than the C atom. Consequently, the rainbow line in the SA plane takes the shape of a 45-degree tilted cusped rhomb, with the longer cusps directed toward the positions of the C atomic strings. From these results, we can conclude that the shape and magnitude of the rainbow lines, which depend on the type and spatial positions of atomic strings, enable precise determination of the structural properties of the SiC crystal using the crystal rainbow theory.

3. CONCLUSIONS

Utilizing the principles of crystal rainbow theory that rainbow lines determine angular distributions of channeled ions, we showed that the shape of these lines depends on the type and spatial positions of atomic strings defining crystal channel and also that it is highly sensitive to the structure of compounds like in the case of the SiC-3C crystal. We demonstrate that by using the crystal rainbow theory, it is possible to determine atomic compositions and crystal structures, which makes this technique highly valuable in the field of crystal characterization.

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