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LOW ENERGY HEAVY ION RAINBOW SCATTERING BY GRAPHENE

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Abstract. We studied low-energy heavy-ion scattering on graphene. Ion trajectories were obtained by numerically solving Newton's equations of motion. To incorporate electron capture processes, we have used time dependent interaction potential. Graphene thermal motion was included by averaging time-dependent interaction potential over the distribution of atomic displacements. We demonstrate that electron capture process does not disrupt rainbow effect.

1. INTRODUCTION

It is known that the rainbow effect accompanies the scattering of light, atom, and ion collisions. Rainbow scattering occurs in ion transmission through thin crystals and nanotubes in the channeling mode [Nešković et al. 2017] and transmission of protons through graphene [Ćosić et al. 2018]. It was shown that the shape of the rainbow pattern contains sufficient information for the determination of the accurate proton-Si interaction potential [Petrović et al. 2015] and proton-cubic crystal interaction potential in general [Petrović et al. 2019, Starčević et al. 2021 and 2023], investigation of the graphene thermal vibrations [Ćosić et al. 2019], and point defects [Hadžijojić et al. 2021]. For these reasons, we investigate how the electron (e^-) capture process affects rainbow scattering in the case of highly charged ion scattering through graphene.

2. THEORY

To study ion transmission through graphene, we have modified the interatomic potential introduced in [Wilhelm et al. 2019], which in atomic units reads

$$V(\boldsymbol{R},t)=\frac{\left(Z_1-Q_{in}+N_{stab}(t)\right)Z_2}{R}\phi\left(\frac{R}{a_2(N_{core}+N_{stab}(t),Z_2)}\right)+\frac{N_{cap}(t)\,Z_2}{R}\phi_{hollow}(R,r_0)+\frac{\left(Q_{in}-N_{stab}(t)-N_{cap}(t)\right)Z_2}{R}\phi\left(\frac{R}{a_1(Z_2)}\right). \quad (1)$$

R is ion-atom distance, ϕ and ϕ_{hollow} are screening functions:

$$\phi\left(\frac{R}{a}\right)=\sum_{k=1}^{3}\alpha_k\exp\left[-\frac{\beta_k R}{a}\right],$$
$$\phi_{hollow}(R,r_0)=\sum_{k=1}^{3}\alpha_k\left(e^{-\frac{\beta_k R}{a_1(Z_2)}}-\frac{\sinh\left(\beta_k r_</a_1(Z_2)\right)}{\beta_k r_</a_1(Z_2)}e^{-\frac{\beta_k r_>}{a_1(Z_2)}}\frac{R}{r_>}\right). \quad (2)$$

Here $r_0=3.42+3.02\sqrt{Q_{in}}$. $\alpha_k=(0.190945,0.473674,0.335381)$ and $\beta_k=(0.278544,0.637174,1.919249)$, $r_<=\min(R,r_0)$, and $r_>=\max(R,r_0)$, $a_1(Z_2)=0.8854/(Z_2/\xi)\text{^}(1/3)$, and $a_2(Z_1,Z_2)=\frac{0.8854}{Z_1^{0.23}+(Z_2/\xi)^{0.23}}$, parameter ξ was modeled according to the Ref. [Wilhelm et al. 2019], N_{cap} is the number of e^- captured into Rydberg states, N_{stab} is the number of e^- stabilized via Auger decay or via extremely fast interatomic coulombic decay (ICD). These are obtained by solving equations [Wilhelm et al. 2019]:

$$\frac{dN_{cap}}{dt}=\lambda(t)\left(Q_{in}-N_{cap}(t)-N_{stab}(t)\right)-\gamma(t)N_{cap}(t),\ \ N_{cap}(-\infty)=0$$
$$\frac{dN_{stab}}{dt}=\gamma(t)N_{cap}(t),\qquad N_{stab}(-\infty)=0. \quad (3)$$

Initially e^- are captured at a rate λ. Close to the membrane they are stabilized by ICD which take place at rate γ, given by the following expression:

$$\gamma(R)=\frac{\gamma_{max}}{1+(R/\gamma_o)^8}. \quad (4)$$

Parameters γ_{max} and γ_o were obtained by fitting the experimental data taken from Ref. [Wilhelm et al. 2019]. Thermal effects were incorporated by averaging interaction potential (1) over the atomic displacements [Ćosić et al. 2018]. The scattering law is a mapping of the impact parameter plane $\boldsymbol{b}=(b_x,b_y)$ to the scattering angle plane $\boldsymbol{\theta}=(\theta_x,\theta_y)$. The differential cross-section σ_{diff} of the scattering process is in the small angle approximation given by the relation

$$\sigma_{\mathrm{diff}}(\boldsymbol{\theta}) = \sum_i \frac{1}{\left|J_{\boldsymbol{\theta}}^{(i)}(\boldsymbol{b}(\boldsymbol{\theta}))\right|}, \tag{5}$$

where $J_{\boldsymbol{\theta}}^{(i)}(\boldsymbol{b}(\boldsymbol{\theta}))$ is the Jacobian of the i-th branch of the map $\boldsymbol{\theta} \to \boldsymbol{b}$. The differential cross-section is infinite along lines

$$J_{\boldsymbol{\theta}}(\boldsymbol{b}(\boldsymbol{\theta})) = 0, \tag{6}$$

called *rainbows*. Note that rainbows dominantly determine the shape of the angular distribution.

3. RESULTS

Descartes's coordinate system was attached to the graphene plane, with the z-axis aligned along the direction of the incident beam. The initial energy of Xe^{32+} was set to 40 keV. Classical equations of motion for thermally averaged potential (1) were solved together with rate equations (3) numerically using Runge-Kutta 8-3 algorithm. In the next step, trajectories were used to determine Jacobian using the Richardson extrapolation method. Rainbow lines were found as the numerical solution of equation (6) using the marching-square algorithm. Figure 1(a) shows the dominant rainbow in the scattering angle plane. The charge state of ions forming this line is indicated by different colors ranging from deep blue to yellow. Obtained rainbow has the shape of a cusped hexagonal line already observed in theoretical calculations of proton transmission through graphene [Ćosić et al. 2018], and experimentally [Watanabe et al. 2024]. Interestingly, e^- capture does not disrupt the rainbow effect. The obtained distribution has a hexagonal shape in the region of small scattering angles and is circular toward the edge. Besides maxima at the zero scattering angle, dominant maxima correspond to the curve in Fig. 1(a). Figure 1(b) shows an exit charge distribution corresponding to the scattering of 100 Xe^{32+} ions with impact parameters lying along a horizontal cross section of the impact parameter plane connecting two neighboring carbon atoms. Notice that most of the ions have exit charge 2. This value is significantly different from the mean charge of the rainbow in Fig. 1(a). This suggests that e-capture processes affect ions forming rainbow less than the others. Using the crystal rainbow theory, one may determine which impact parameters correspond to the observed scattering angles. Hence, one may determine how e^- capture depends on the ion impact parameter. Tilting graphene displaces rainbow line, which could enable scanning of the entire graphene impact parameter plane in this way [Ćosić et al. 2021].

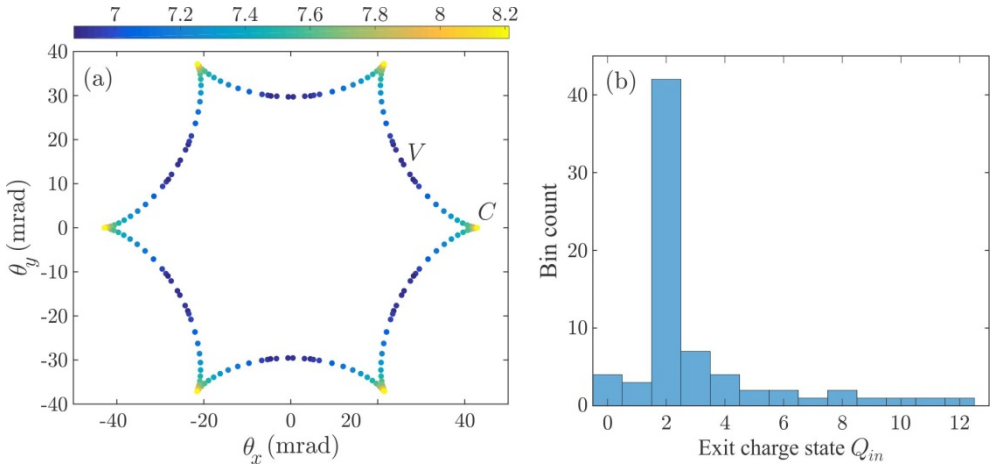

Figure 1: (a) Rainbow line in the scattering angle plane generated by the 40 keV Xe^{32+} ions scattered by graphene. The corresponding exit charge state colors are rainbow. (b) Exit charge state distribution of 40 keV Xe^{32+} ions with impact parameters along a line in the impact parameter plane connecting the center of a graphene hexagon and a midpoint between two adjacent C atoms.

Being structurally stable, rainbow shape is noise immune, and could be used to determine more accurately or reduce the number of model parameters. Note that maximal difference of the rainbow exit charges occurs for points marked in Fig. 1 by *C* and *V*. Subsequent trajectory analysis showed that distance of the corresponding impact parameters from the graphene hexagon center are 79.9 pm, and 83.4 pm respectively. Therefore analysis of the rainbow shape provides insight in the neutralization process at picometer scale.

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