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The investigation of the graphene atom thermal vibrations using forward rainbow scattering

This paper reports the findings of the investigation of graphene atom thermal vibrations using angular patterns of transmitted non-neutralized 5-keV protons. The static proton - graphene interaction potential was constructed using Doyle-Turners expression for the proton-carbon interaction potential. The effect of the thermal vibrations was incorporated by averaging the static proton-graphene interaction potential over the distribution of the atom thermal vibrations. Covariance matrix of atom displacements was modeled according the Debye theory, and calculated using Molecular Dynamic approach. Trajectories of the protons, obtained by numerical solution of the corresponding Newton's equation of motion, were used for construction of the mapping of the impact parameter plane to the transmitted angle plane. Singular lines of this mapping –called the rainbow lines –were constructed, and their evolution with the change of the graphene sample tilt angle was investigated.

The shape of the transmitted angular yield and its evolution with the change of the tilt angle was explained by the introduced singularities. Rainbow lines formed by protons experiencing the close collisions with the carbon atoms were modeled by elliptical lines which parameters were found to be very sensitive to the structure of the covariance matrix. Moreover, a procedure was developed which enables extraction of the covariance matrix from the corresponding rainbow patterns.

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