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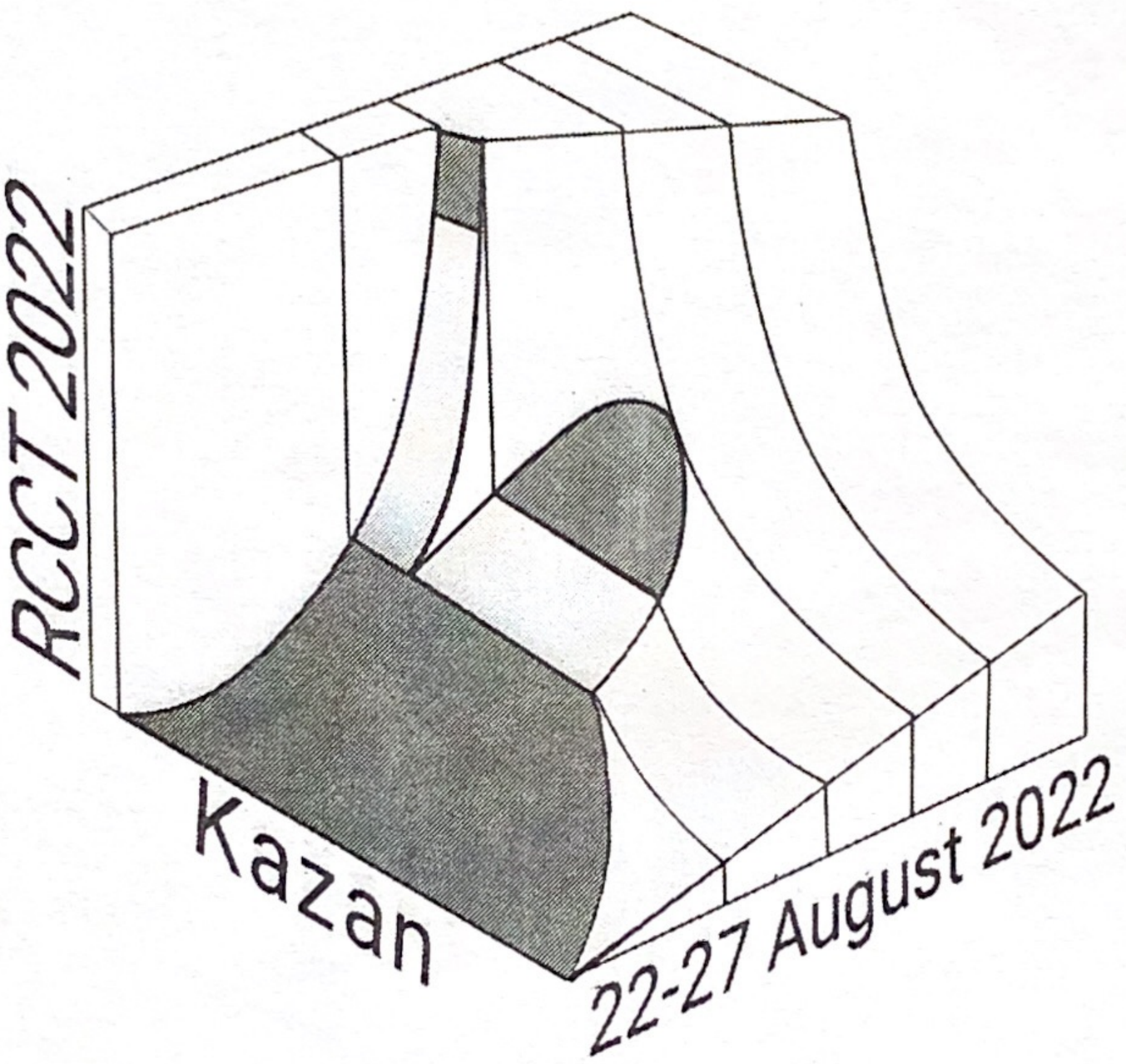

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BOOK OF ABSTRACTS

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CRYSTAL NUCLEATION IN AMORPHOUS SYSTEMS: UNIVERSAL SCALING RELATIONS

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One of the most popular scenarios for the crystallization of supercooled liquid is the process of crystal nucleation and the subsequent growth of crystalline nuclei. Depending on how supercooling was initially achieved and under what conditions the subsequent crystallization of a supercooled liquid (or an amorphous solid) occurs, it is possible to obtain a material whose structure, and, consequently, the physical and mechanical properties can be very diverse. In this regard, understanding the initial stage of crystallization as a phase transition seems to be very necessary and important.

Crystal nucleation in atomistic/molecular systems occurs, as a rule, on nanometer spatial scales; the critical size of a crystalline nucleus under certain conditions can be only a few tens of particles. As a result, wide opportunities in research in this area are opening up for methods of molecular dynamics simulations. The results obtained using both classical and quantum mechanical molecular dynamics simulations not only complement the data of traditional experiments on microscopy, diffraction, spectroscopy, etc., but also allow one to reveal completely new patterns in the processes of crystal nucleation.

In this work, we will show that the temperature dependences of the rate characteristics of crystal nucleation processes are described by universal scaling relations [1–6].

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