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Disclination formation in two-dimensional dense systems of hard and soft disks

Hard objects can behave differently from the objects/particles that are interacting through soft potential. The main difference is that soft interacting particles can store potential energy accommodating at the same time their positions. Hard interacting particles possess no potential energy and their arrangement is fully according to the entropic and geometry conditions. The excluded volume which is determined by the shape of the particles plays here a decisive role. Still all the consequences of these conditions are not fully examined. In this presentation we show the behavior of the very dense system of hard disks in comparison to the system made of soft disks. Using Event Driven molecular dynamics we observe in an initially perfect hexagonal arrangement a strong tendency of disclination formation, which we also call as minicracks. Minicracks are the places in the system where particles close to each other are situated on the square lattice. This concerns only two rows of particles. Beyond this area the arrangement is hexagonal. Upon evolution the free space initially present in between particles diffuses to the minicrack areas, although some part must be still present, otherwise the system will be blocked. At the same time the average distance between particles diminishes. This is purely an entropic effect which is not observed in soft interacting particles. We argue that such a free space diffusion into disclinations in harder objects systems can tell on the formation of large cracks, since the minicracks play the role of the seeds for larger crevices. Cracking is a big technological problem. In thin film, for instance, cracking spoils surface properties. It has been already observed that under electron or ion bombardment, even if such the interaction at the surface is rather point like, a large crack develops which ruins the regularity of the surface. We speculate whether the free space diffusion mechanism can be the driving force for spoiling such films. The possible physical reasons why free spaces diffuse to minicracks have been also discussed.

Summary

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