2020 Summer Physics Research

Going Against The Grain

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Howdy, neighbor grains!

Crystal grain motion determines many material properties of crystalline solids. Observing the particle-scale mechanisms that cause grain motion in colloidal crystals can help us better understand the physics that underlies material properties. Previous groups have observed grain rotation in colloidal crystals; however, in these experiments the crystal grains were not embedded in a surrounding crystal, which is known to influence behavior **[1].** This summer we investigated grain rotation of neighboring pairs of embedded colloidal crystal grains.

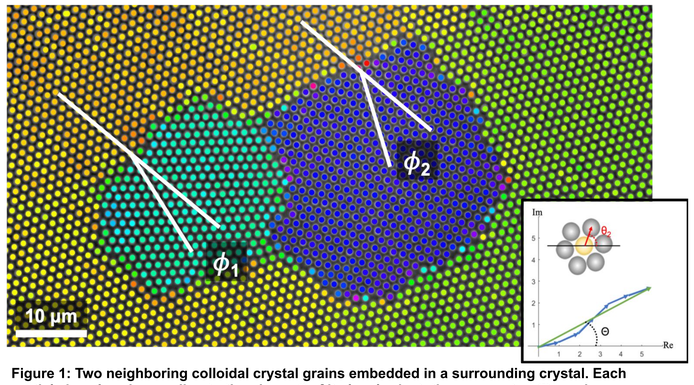

Figure 1: Two neighboring colloidal crystal grains embedded in a surrounding crystal. Each particle is colored according to the phase Θ of its local orientation parameter, Ψ_6 as shown in the inset and defined by equation (1). Misorientation angles, φ_n, measure the difference in lattice orientation between two grains that share a grain boundary as shown by the white lines marking the crystal axes.

An optical blasting technique previously developed in the Gerbode lab was used to create neighboring, embedded grains **[2]**. This summer we analyzed data from a single experiment with two neighboring grains embedded in a larger surrounding grain (Fig. 1). Our analysis shows not only that grain rotation can occur for embedded colloidal crystals, but also that grains can split apart into subgrains (which we refer to as "granules") that rotate independently in opposing directions. These results deviate from previous theories that treated grain rotation as rigid body rotation **[3][4].** We analyzed the total free energy of the grain boundaries before and after the split and found that grain splitting and rotation reduces the total energy of the system.

Characterizing the system

Grains are characterized by their uniform crystal lattice orientation. This uniform orientation changes at the interface between distinct grains, known as grain boundaries. Grain boundaries are areas of local disorder where the orientations of the bordering grains do not align. Because grain boundaries are more disordered and less closely packed, they increase the free energy of the crystal.

The misorientation angle, φ, is the difference in angles between neighboring crystal orientations. In Figure 1, φ_1 is the difference in orientation of the surrounding grain and left embedded grain as illustrated by the angle between the longer and shorter white lines—these white lines align with the orientation of the grains.

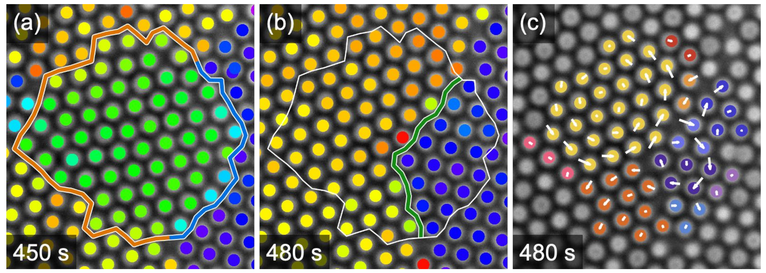

Figure 2: Visualizing grain splitting and rotation. (a) The grain boundary surrounding the embedded grain just before the split is made up of two segments, highlighted in orange and blue. These two segments correspond to the two different misorientation angles relative to the two crystals within with this grain is embedded. Particle color indicates Ψ_6 phase. (b) After the split, a new grain boundary segment (green) is formed. The outline of the grain just before the split is shown in white. (c) Grain splitting occurs via the rotations of individual granules. Each granule is shown with a distinct color, and the individual particle displacements from their positions just before the split are overlaid in white.

We quantify local crystal orientation by considering for each particle the complex order parameter Ψ_6 shown in equation (1)

$$\Psi_6 = \frac{1}{N}\sum_{n=1}^{N} e^{i6\theta_n} \equiv |\Psi_6|e^{i\Theta} \qquad (1)$$

where N refers to the number of nearest neighbors, and θ_n represents the angle each nth particle makes with the horizontal axis as marked in the inset of Fig. 1. The resulting angle of the vector sum is called Θ, and we use this value as the primary method for quantifying local crystal orientation.

Why did grain splitting and rotation occur?

Using a light microscope, images were collected at a rate of two frames per minute. We observed grain splitting and rotation in the smaller, left grain, as shown in Fig. 2, where the particles are colored according to the phase of Ψ_6. The grain boundary surrounding the left embedded grain is shown in Fig. 2(a), divided into orange and blue segments to indicate regions with different misorientation angles. The same region is outlined in white in Fig. 2(b) to indicate the original location of the grain before the split.

We found that rather than rotating as one or even two rigid bodies, the particles in the grain rotate as many smaller rigid "granules." Fig. 2(c) shows the particles colored by these granules, with the displacement vectors of each particle overlaid that show local rotation by granule.

Figure 3 shows the average Ψ_6 phase of each granule as a function of time, plotted in dotted lines. Each granule rotates in a direction to match the orientation of the grain it then joins. The average Ψ_6 phase for the particles in these resultant grains are plotted in bold. Together, Figures 2 and 3 demonstrate that the original left embedded grain splits into two grains by first forming multiple rigid granules that rotate independently.

For interfaces with low-angle grain boundaries, the interfacial energy per unit length can be found using the Read-Shockley equation, given by equation (2)

$$\gamma = \gamma_0 \phi\,(A - \ln\phi) \qquad (2)$$

where φ is the misorientation angle, and γ_0 and A are constants dependent on material properties of the crystal **[5]**. For this system, A has been determined to be approximately 1 **[2]**. We computed the interfacial energy per unit length and total interfacial energy and discovered that grain splitting and rotation lowered the total free energy of the region we considered to approximately 39% of the original amount, as illustrated in Fig. 4.

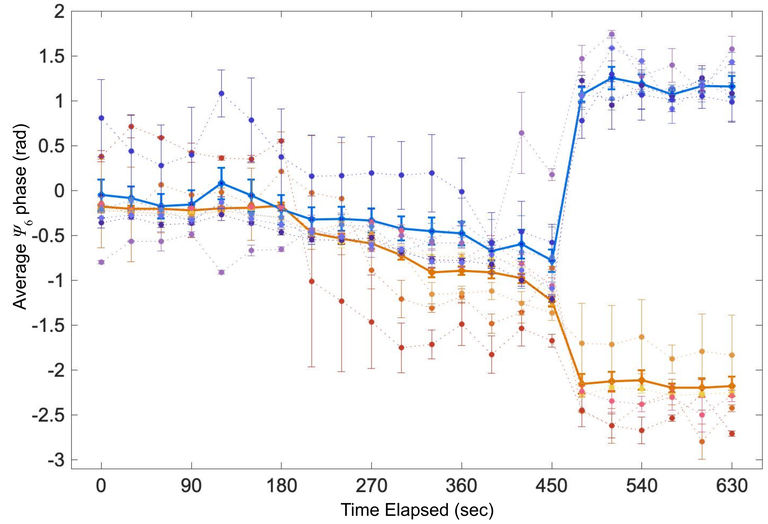

Figure 3: Average Ψ_6 phase plotted by granule (dotted) and grain (solid bold) show splitting and independent rotation. Grain 1 and its constituent granules are shown in orange, with grain 2 in blue.

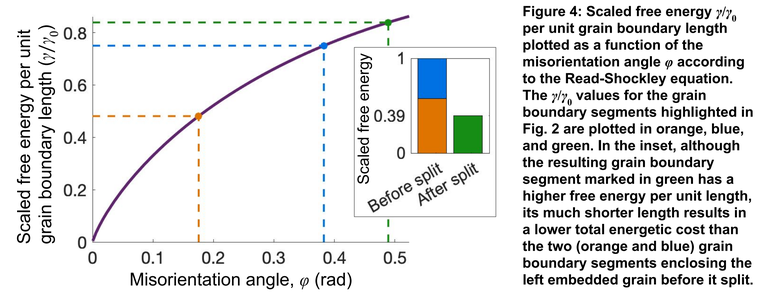

Figure 4: Scaled free energy γ/γ_0 per unit grain boundary length plotted as a function of the misorientation angle φ according to the Read-Shockley equation. The γ/γ_0 values for the grain boundary segments highlighted in Fig. 2 are plotted in orange, blue, and green. In the inset, although the resulting grain boundary segment marked in green has a higher free energy per unit length, its much shorter length results in a lower total energetic cost than the two (orange and blue) grain boundary segments enclosing the left embedded grain before it split.

Conclusions and Future Work

Our analysis has demonstrated that not only do colloidal crystal grains rotate, they can also split by breaking into rigid granules that rotate independently. Furthermore, our Read-Shockley analysis has shown that this grain splitting and subsequent rotation lowers the free energy of the system by reducing the overall cost of grain boundaries. These results suggest that grain splitting, which is not currently described in grain boundary theories, may play an important role in crystal grain motion, perhaps particularly for small grains. Future studies could investigate the importance of grain size, misorientation angles, and other physical parameters in determining whether grains will split.

References

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