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Differential Diffusion as a Root Cause of Cracking of Protein Crystals

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Protein crystals are nanoporous materials important for high resolution structure determination of proteins via X-ray diffraction. Additionally, their nanoporous character has made protein crystals useful for other applications including separations, catalysis and drug delivery. As materials, protein crystals contain both an ordered array of protein molecules and a disordered aqueous phase, which permeates the crystal inside the pores. The combination of order and disorder confers on the crystals interesting structural, thermal and transport properties. Here we focus on the transport of molecules through the pores and how such transport affects the structural integrity of the crystal. During their use, protein crystals are often subjected to solution changes that can cause damage, including cracking. When a crystal is transferred between two solutions of different composition, solutes and water molecules may enter and/or leave the crystal via its pores. The severity of cracking correlates with differences in both concentration and diffusibility of the entering and exiting molecules. The observed behavior motivates a model in which the key aspect of crystal cracking is differential diffusion of solutes, which causes an osmotic pressure induced stress on the crystal beyond its elastic limit. The result points to some simple guidelines for improved crystal handling.

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