Oral Contributions

[MS39] Crystallisation and crystal treatment
Co-Chairs: Terese Bergfors (SE), Jose Gavira (ES)

[MS39-01] The effect of impurities and solvent viscosity on protein crystal growth.

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Despite the advent of structural genomics projects, obtaining diffraction quality protein crystals still constitutes a major bottleneck in the gene-to-structure pipeline. In this talk we will start by giving a general introduction on protein crystal growth mechanisms and step dynamics. As protein solutions are often contaminated by species of micro-heterogeneous (dimers, trimers, oligomers, partially unfolded, domain swapped species,…) or foreign origin (contaminant remnants from purification,…) we will then focus on impurities and their role in protein crystal growth. Firstly we will show that by simply departing from well-established purified protein model systems, one can obtain unconventional and highly complex protein crystals with nontrivial growth mechanisms [1,2]. Secondly we will report on our analysis of lysozyme crystals growing from purified and contaminated solutions. It was found that the morphology and step dynamics of spiral hillocks are less affected by the presence of impurities in the growth solution as compared to steps generated by 2D nucleation [3,4]. We will discuss the failure of the Cabrera−Vermilyea (CV) step pinning model to reproduce the observed elementary step kinetics. As such, we developed theoretical time-dependent impurity models based on Bliznakov kinetics assuming Langmuir adsorption on the one hand and clustering of impurity molecules on the surface on the other hand. The last phenomenon is corroborated by our in situ experimental atomic force microscopy observations. Our observations as well as our theoretical models are supported by Monte Carlo simulations. To conclude we will discuss the role of viscosity, a fundamental solution characteristic which is used as a proxy measure of the effects of the medium on the rates of transport processes and chemical transformations in solution [5]. We establish that the rate constant for molecular attachment is proportional to the reciprocal viscosity and to the diffusion coefficient. This observation agrees with the basic theories of chemical kinetics and may serve as a benchmark for future studies in solutions with frequency-dependent viscosity.

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[4] Mike Sleutel and Alexander E. S. Van Driessche (2013), Crystal Growth & Design 13, 688-695.
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