

Poster Presentation

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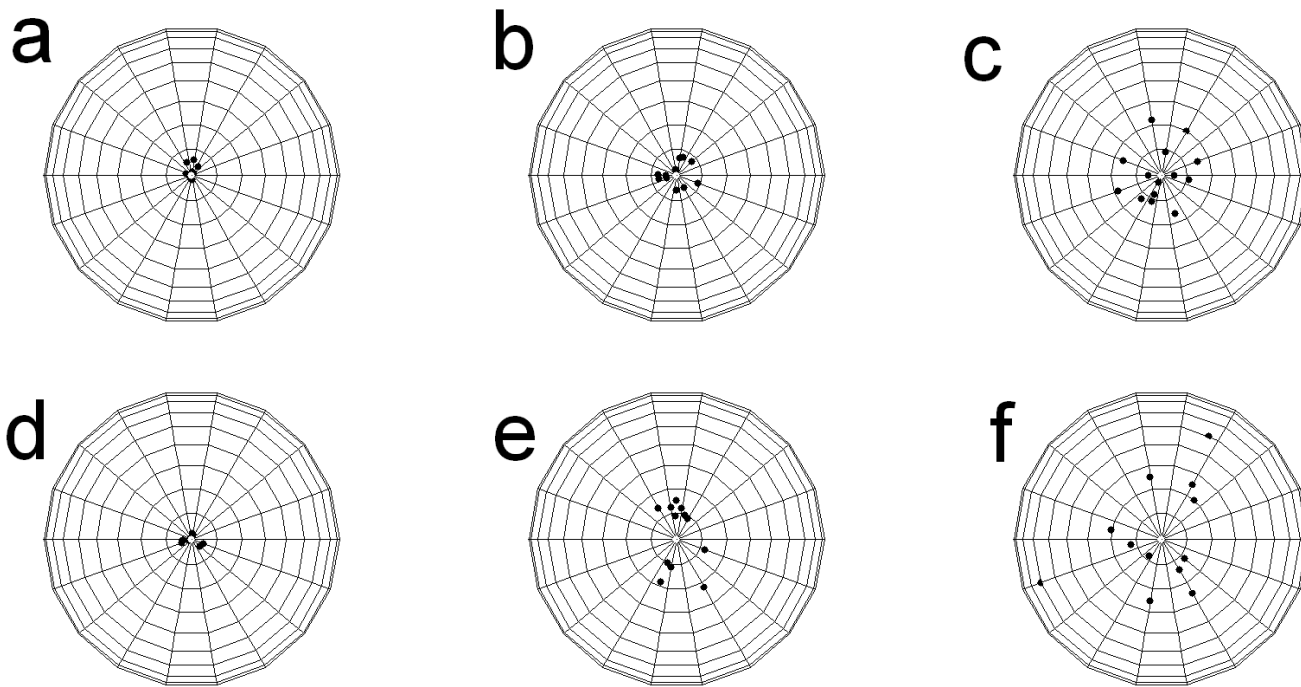
Particle orientation from distribution of explosion fragments in XFEL experiment

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In many XFEL experiments small objects with unknown orientations are introduced into the x-ray beam. However, understanding the measured quantities it would be desirable to know their orientations. This is the situation in the case of single-molecule imaging one of the main target areas of X-ray free-electron lasers. Here, the solution to the orientation problem is based on the possibility of orienting the large number of low-counting-statistics 2D diffraction patterns taken at random orientations of identical replicas of the sample. This is a difficult process and the low statistics limits the usability of these methods and ultimately it could prevent single-molecule imaging. We suggest a new approach, which avoids the use of the diffraction patterns. We propose to determine the sample orientation through identifying the direction of ejection fragments. The orientation of the sample is measured together with the diffraction pattern by detecting some fragments of the Coulomb explosion. We show by molecular-dynamics simulations that from the angular distribution of the fragments one can obtain the orientation of the samples [1]. The figure shows the distribution of heavy atoms coming from different depth of the sample (upper panel homogeneous, lower panel inhomogeneous model samples, and left to right is heavy atom at the outer boundary, halfway to center and at the center).

[1] Z. Jurek, G. Faigel, *EPL*, (2013), 101, 16007



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