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OASIS-2004 and Cr Radiation Combined for Enhanced In-House SAD Phasing. Cheng Yang¹, Haifu Fan², Xiaodong Su³, Jiawei Wang², Yuanxin Gu², Yuhe Liang³, James W. Pflugrath¹, Joseph D. Ferrara¹ Rigaku/MSC Inc. Spring, TX, USA; ²Inst. of Physics, CAS, China; ³Peking Univ., China.

The recent successes of SAD phasing using an in-house Cr radiation (2.29 Å) source have demonstrated that softer radiation is a useful tool to extract the weak anomalous signals from scatterers like sulfur and selenium. However, to make Cr-SAD phasing robust, it is essential to have a good algorithm to break the intrinsic phase ambiguity. Many of the approaches in use now have had reasonable success. In these approaches, like solvent flattening, initial phases are based on discrimination of the Sim distribution only. A direct methods procedure (OASIS) was proposed in the 1980s to break the phase ambiguity in SAD and SIR phasing. This method uses the product of the Sim and Cochran distributions to discriminate the phases. Recent results reveal it can lead to better initial phases and consequently to better electron-density maps. The newest version, OASIS-2004, includes an algorithm for tuning the scaling factor associated to the lack-of-closure error and partial-structure iterative phasing. In this report, we will show examples of SAD phasing by combining OASIS-2004 with Cr SAD data. A few examples of SAD-phasing by using OASIS-2004 and synchrotron data are also discussed.