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New Developments in Chromium Phasing. C. Yang, J.W. Pflugrath, A. Yamano, H. Kawasaki, H. Yamazaki, C.N. Stence, D.A. Courville, J.D. Ferrara*, Rigaku/MSC, Inc. 9009 New Trails Dr., The Woodlands, TX 77381.

Single-wavelength anomalous dispersion (SAD) has become a popular method of phasing macromolecular crystal structure. Recent results from our Sulfur-SAD experiments [1] have demonstrated that both less redundancy and lower resolution data is required when the data are collected using Cr $K\alpha$ radiation compared to the highly redundant and high resolution data that is needed when Cu $K\alpha$ radiation is used. In our original work we have potential to collect weak anomalous signals using Cr $K\alpha$ radiation in collecting weak anomalous scattering. In addition, long wavelength radiation may increase the diffraction signal for small crystals because scattering efficiency is proportional to λ^2 . Finally, longer wavelengths also improve the spot resolving power. Diffraction maxima of unit cells over ~ 600 Å can be resolved at a crystal-to-detector distance of 175 mm. These results indicate that Cr $K\alpha$ radiation has become a good alternative to Cu $K\alpha$ radiation for an in-house source for macromolecular crystallography.

However, many proteins have fewer sulfur atoms, hence a weaker anomalous, than the thaumatin and trypsin crystals we used as our test cases. Thus, a Cr FR-E system was assembled using a Cr anode installed in an F-RE SuperBright and the original Cr optic. It was found that only 180° of data from a crystal of glucose isomerase was needed by SOLVE to find the sulfur positions. The experimental electron density map is of sufficient quality that the structure can be built automatically by RESOLVE at 3.0 Å resolution. After the VariMax Cr optic became available, both Cr MicroMax-007 and Cr RU-H3R systems were assembled and these systems can provide similar flux to the Cr FR-E system using the older optic. Some difficult cases were solved by using the data collected from these new systems.

[1] Yang C., Pflugrath, J.W., Courville, D.A., Stence, C.N., & Ferrara, J.D.. Acta Cryst. (2003), D59, 1943-1957