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**Supporting information for article:**

# Exploring the impact of incoherent Compton scattering on X-ray pair distribution function analysis of disordered materials

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# Table of Figures

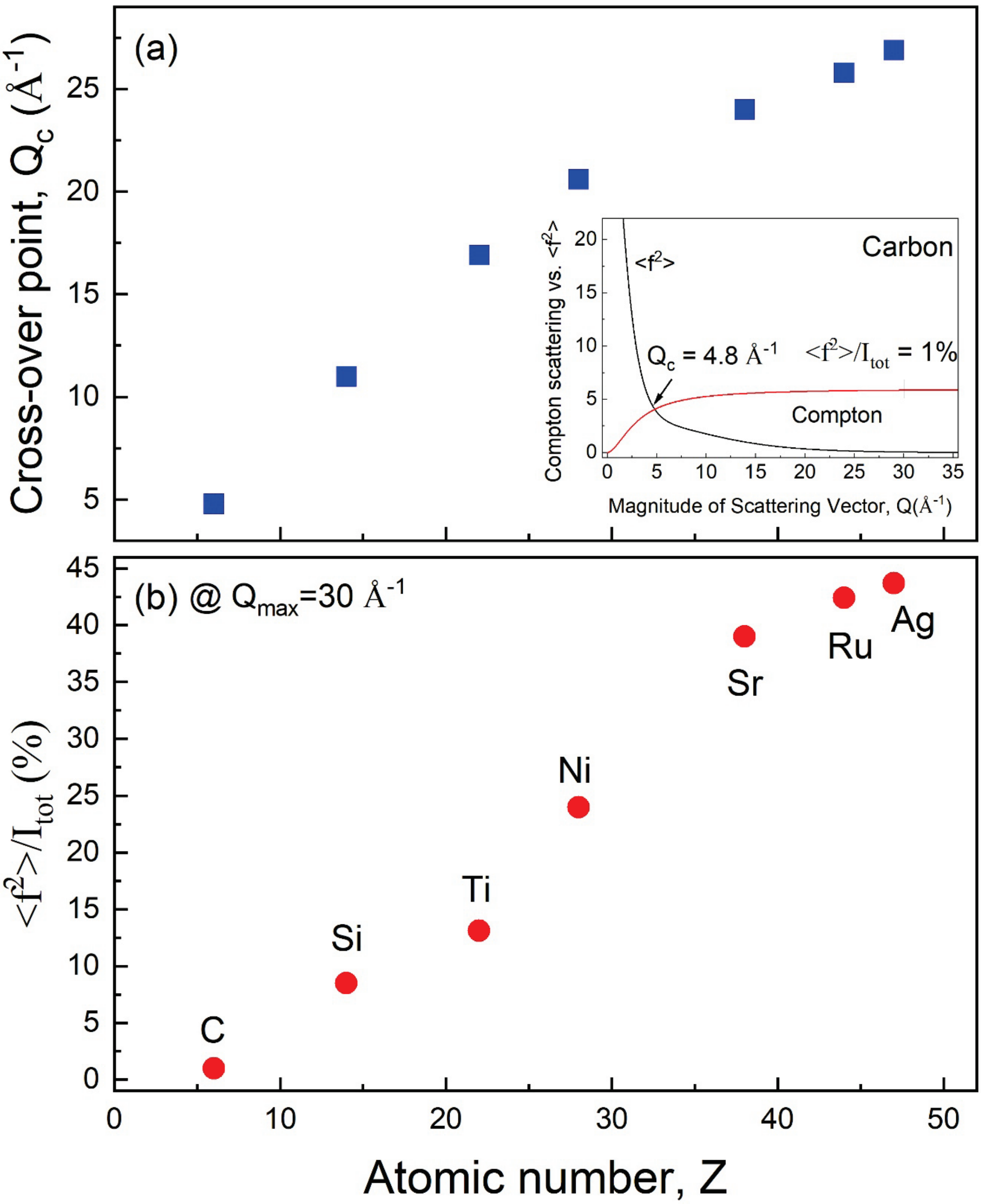


Fig. S1. (a) Cross-over point, $Q_c$ between Compton intensity and $<f^2>$ as a function of atomic number, Z. The inset shows a comparison of Compton and atomic form factor of Carbon. The cross-over point $Q_c$ and $<f^2>/I_{tot}$ at Q = 30 Å$^{-1}$ are marked. (b) The ratio of $<f^2>$ to the total intensity $I_{tot}$ at $Q_{max}$ = 30 Å$^{-1}$. For light elements such as carbon and silicon, elastic scattering estimated by $<f^2>$ is less than 10% of the total intensity.

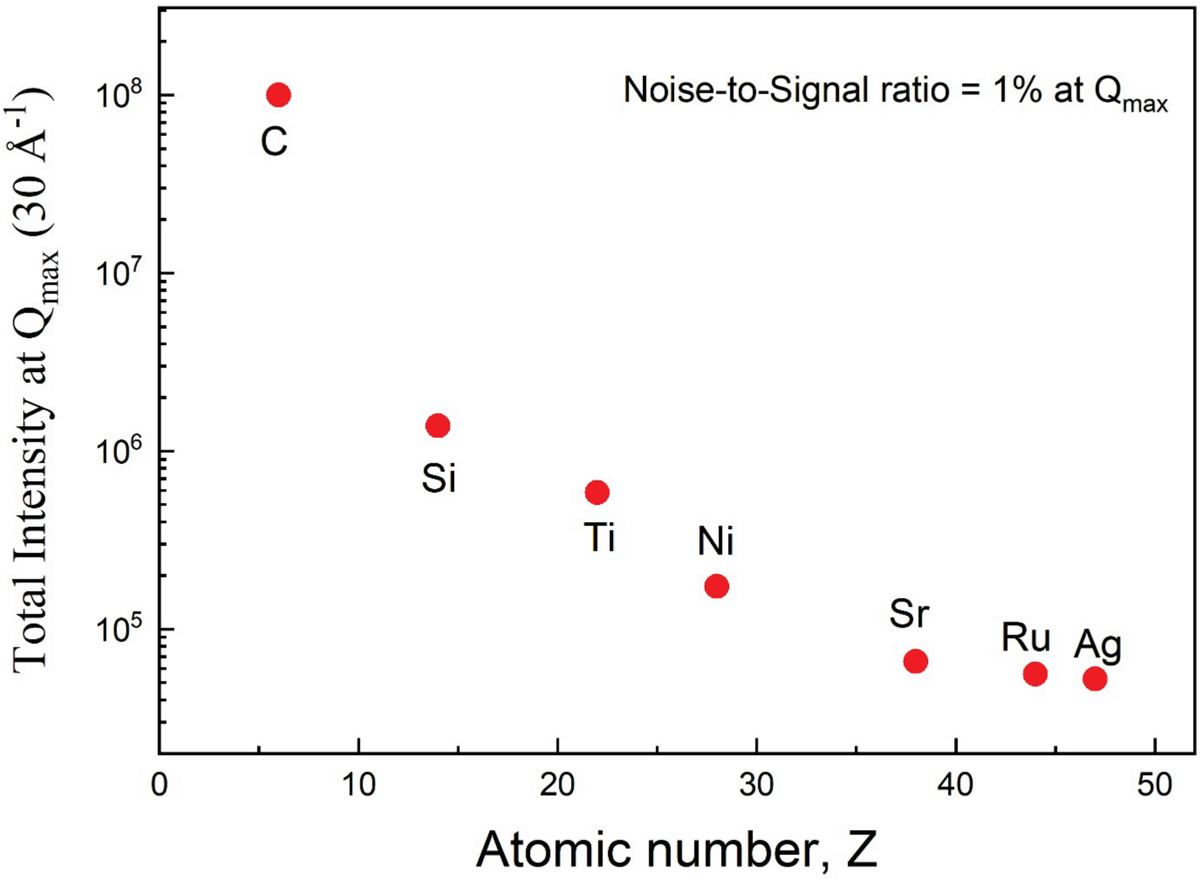


Fig. S2. Total intensity $I_{tot}$ required to achieve a noise-to-signal ratio of 1% at $Q_{max}$ = 30 Å$^{-1}$ based on $\langle f^2\rangle/I_{tot}$ shown in Fig. S1(b) as a function of atomic number, Z. For lighter elements, much higher counts are measured. Beyond strontium, the slope of $I_{tot}$ with Z becomes weak.

In the simulation studies we tested three cases with total intensities 7500, 30,000, and 120,000 counts at $Q_{max}$ = 35 Å$^{-1}$. In the Fig. S3, simulated XRPD intensity (elastic and Compton scattering) shown in (a) is re-scaled with scale factor of 310 to obtain total intensity of $I_{tot}$ = 7,500 at $Q_{max}$ = 35 Å$^{-1}$ (Fig. S3(b)). For a given ratio $\langle f^2\rangle/I_{tot}$=0.33 at $Q_{max}$ (35 Å$^{-1}$), the corresponding elastic scattering $\langle f^2\rangle$~7500×0.33≈2500 counts, and the intensity of Compton scattering is about 7500×0.67≈5000 counts, respectively. And then, random noise is added using Poisson statistics based on rescaled intensities of elastic and Compton scattering. After rescaling, the N/S ratio given by $\sqrt{I_{coh}+I_{inc}}/\langle f^2\rangle$ is $\sqrt{7500}/2500 = 3.4\%$ . Similarly, Fig. S3(c) shows the case with total intensity of 30,000 counts (scale factor 1240). Here, $\langle f^2\rangle$ is about 10,000, and the Compton intensity is 20,000 respectively. Thus, the N/S will be about 1.7%.

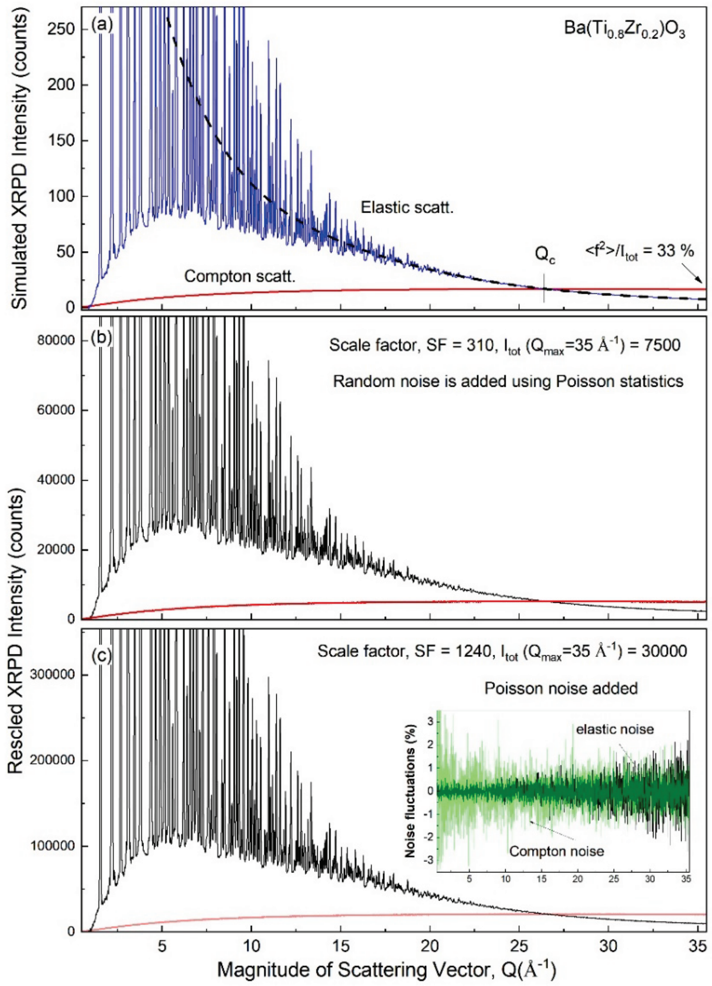


Fig. S3. (a) A simulated x-ray elastic diffraction pattern and Compton scattering of $Ba(Ti_{0.8}Zr_{0.2})O_3$. The ratio of $\langle f^2 \rangle$ to $I_{tot}$ is 0.33 at $Q_{max}$ = 35 Å$^{-1}$. (b) Re-scaled intensities of elastic and Compton scattering with scale factor of 310. Total intensity at $Q_{max}$ = 35 Å$^{-1}$ is 7,500. (c) Re-scaled XRPD intensity with SF = 1240 to have total intensity of 30,000 at $Q_{max}$ = 35 Å$^{-1}$. After re-scaling random noise is added following Poisson statistics. The inset shows noise fluctuations in elastic and Compton scattering.