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Dynamics of Electron Beam Channeling in Single Atomic Column and in Crystals

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Manifestation of channeling effects in quantitative interpretation of atomic-resolution measurements made using scanning transmission electron microscope (STEM) has been observed in imaging and spectroscopic data [1-3]. Here, channeling refers to the path of the electron beam along atomic columns in a crystal. A feature common among STEM probe path in crystals of many different elemental compositions and crystal structures, is oscillation in intensity of the electron beam along one atomic column of a crystal. The oscillations are observed before any significant portion of the intensity is seen to accumulate on neighboring columns, which has been reported in Si [110] and Si [211] [4,5], and shown in Figure 1(a). That oscillations in intensity occur independently of scattering effects from neighboring columns was confirmed by simulating beam behavior in hypothetical individual isolated atomic columns. The physical changes in the STEM probe that lead to oscillation in intensity were expected to be the same in crystals and isolated columns because of the observed similarity in the characteristics of the oscillations, frequency and magnitude. In fact, the level of difference between characteristics of intensity oscillations in crystal and isolated column was systematically outlined based on crystal features, elemental composition and lattice parameters, see Figure 1(b), with an almost exact match shown in Figure 1(c).

The study was based on the multislice theory by Cowley and Moodie [6] and beam behavior was simulated using the code by Kirkland [7]. The multislice theory simulates a 2D wave function, which models the STEM probe in the plane perpendicular to the optic axis before the probe scatters from the specimen, and then simulates the 2D wave function at subsequent planes, also perpendicular to the optic axis, during propagation through the specimen for the entire depth of the specimen. The multislice algorithm thus allows an insightful view of a highly focused electron probe changing as it transmits through a crystal, scattering repeatedly from planes of specimen's atoms and slightly molding itself each time.

Examination of the probe during propagation through a single atomic column revealed that there are two types of physical changes that lead to oscillations in intensity during transmission through a single atomic column [8]. One is due to the movement of the probe, occurs without the presence of any scattering potentials, and leads to fluctuations in the intensity of the STEM probe propagating in vacuum. This is change in the relative phase shifts of the different k-components of the STEM probe. The other physical change results from scattering of the probe by the specimen's atoms. This is change in the angular distribution of the probe. As can be expected, when changes in the angular distribution dominate probe behavior, the characteristics of the intensity oscillations depend heavily on the specimen's elemental composition [8].

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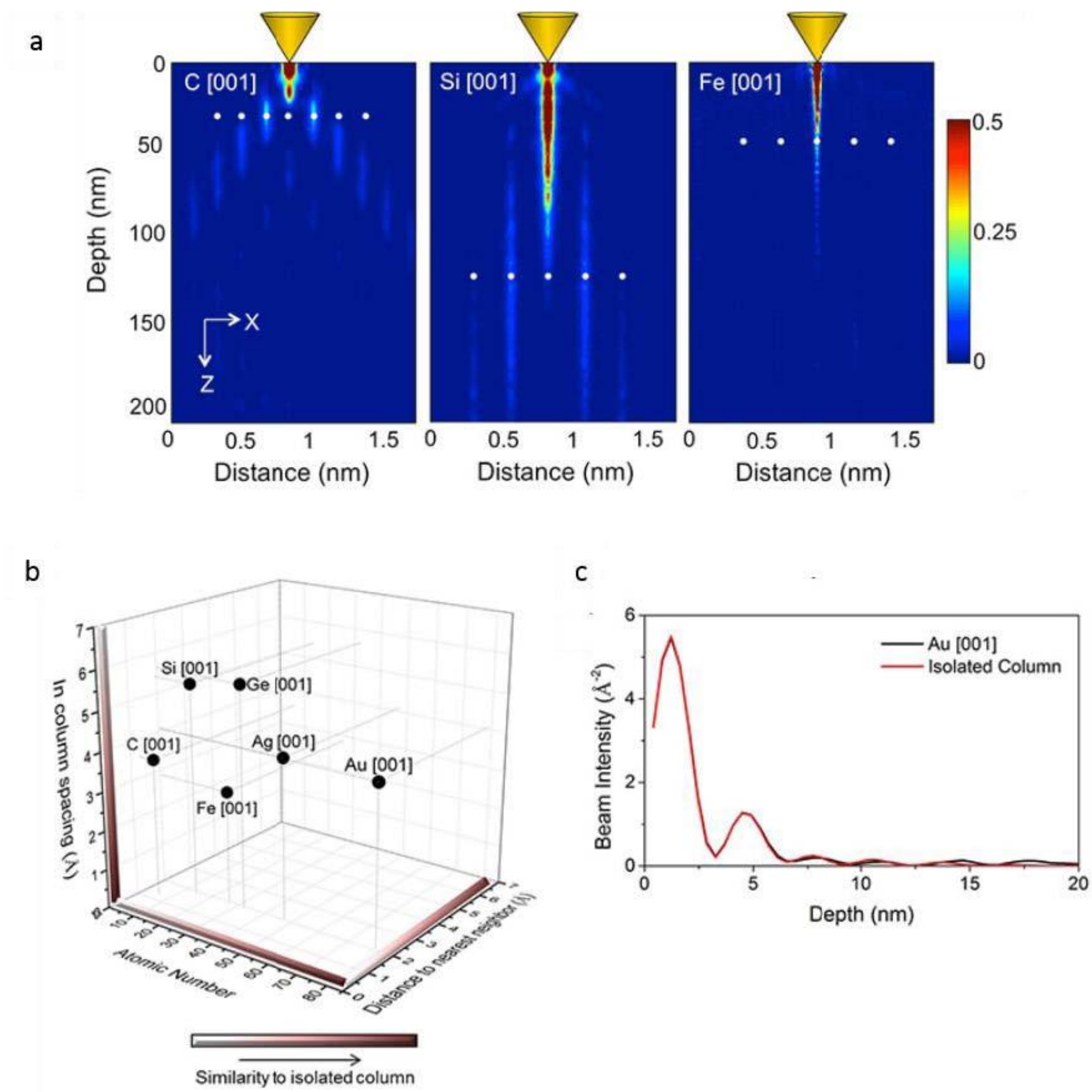

Figure 1. (a) 2-D beam intensity depth profiles in crystals of diamond [001], Si [001], and α Fe [001]. The cross-sections are parallel to (100) plane. The solid circles mark positions of atomic columns. **(b)** Diagram summarizing the effect of crystal features on similarity between beam oscillations in atomic column in crystals and in isolated columns. **(c)** Beam intensity depth profile in Au [001] crystal and in an isolated column of Au. An E_0 = 100 keV and α_{obj}= 25 mrad aberration-free STEM probe is used in (a,c). Figure adapted from [8].

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