Unique Atomic Structure of Copper as the Origin of Fracture

In order to gain fundamental knowledge about the origin of fracture (trigger site) by observing structural changes at the moment of fracture of metals, laser impact fracture of copper was observed using a time-resolved technique. It was found that 117 ns after laser irradiation, there existed a "short-range-disorder-only" state, which was locally disordered and kept an ordered structure over a long distance. This state can be reproduced by a model in which all copper atoms in the fcc structure are randomly displaced in three dimensions by 10% relative to the nearest-neighbor bond distance. The "short-range-disorder-only" state in a small region, such as around the crack tip, is considered to be the starting point of fracture.

Metals are widely used as infrastructure materials in bridges, buildings, automobiles, airplanes, and rockets. Therefore, understanding their fracture processes is crucial for controlling mechanical properties and designing safety margins for structural materials. It is widely known that when mechanically loaded with increasing strain at slow strain rates such as 0.1–1.0 s^{-1}, common metals undergo a static transition from elastic to plastic deformation due to dislocation formation and their movement. However, the moment of plastic deformation leading to fracture, which is a dynamic change corresponding to high strain rates exceeding 10^6 s^{-1}, is expected to progress within milliseconds [1, 2], and the mechanism has not been elucidated. In this study, we performed time-resolved dispersive X-ray absorption fine structure (dispersive XAFS, DXAFS) observation of the laser impact fracture of copper in order to obtain fundamental knowledge about the origin (trigger site) of fracture by observing the structural change at the atomic level at the moment of fracture of the metal.

A 5 μm-thick polycrystalline copper foil was irradiated with a YAG laser (power: 1.3 J, wavelength: 1064 nm, pulse duration: 10 ns), and the process of copper fracture was measured using time-resolved DXAFS and X-ray diffraction (XRD). The XAFS spectra [Fig. 1(a)] [3] show the disappearance of the extended XAFS (EXAFS) oscillation after 117 ns of laser irradiation, which indicates the disappearance of the local structure (short-range order: SRO) of copper. On the other hand, in XRD [Fig. 1(b)], a shift of the diffraction peak from the {111} plane of fcc copper due to the compression by laser irradiation was observed in the early stage, but the peak was still clear 208 ns after the laser irradiation. This indicates that there is no significant change in the amorphization or crystallite size, indicating the presence of long-range order (LRO). These results of time-resolved DXAFS and XRD measurements, as well as transmission electron microscopy (TEM) observations of the specimens collected after laser irradiation, indicate that the laser-irradiated copper existed in a state that maintains the fcc structure during the destruction process, eventually becoming nanoparticles of a few nm. In the process, at 117 ns and 317 ns after the laser irradiation, XAFS showed a disorder in the local structure, while XRD showed the existence of long-range order. This means that there is a disordered structural state only locally, while the long-range ordered structure is preserved ("short-range-disorder-only" state). We constructed an inhomogeneous structure model in which the atomic structure is locally and inhomogeneously disordered, and calculated XAFS and XRD for the model using FEFF8, which is an automated program for *ab initio* multiple scattering calculations of XAFS, and the original software, respectively. In the randomly displaced XAFS spectra [Fig. 1(a)], the EXAFS oscillation of the spectrum disappeared with increasing displacement and reproduced the experimental data well. Similarly, the normalized peak of the calculated XRD spectra [Fig. 1(c)], which was obtained by considering random displacement, remained almost unchanged when the amount of displacement was varied, in good agreement with the experimental XRD results.

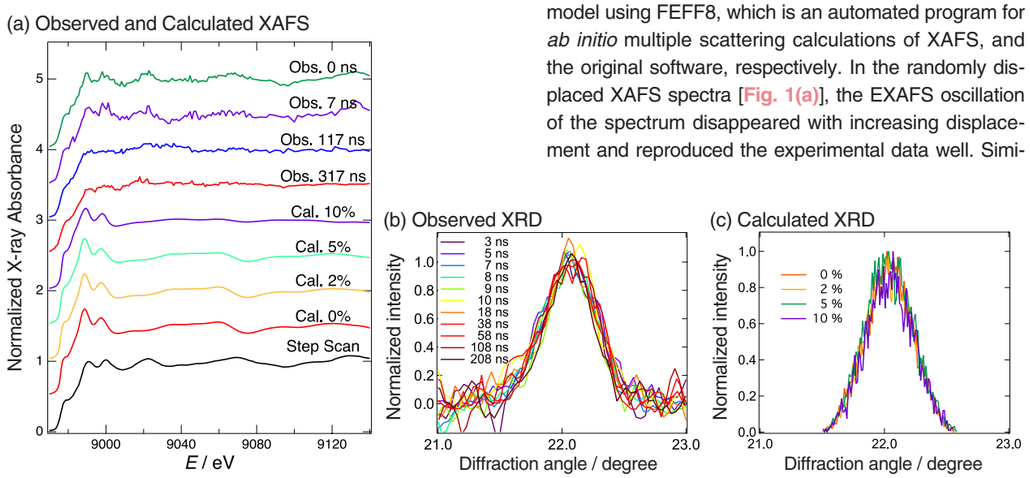

Figure 1: Comparison of calculated XAFS and XRD with experimental results for copper. **(a)** XAFS spectra at each delay time for DXAFS and Step Scan, and at 0–10% random displacement of the atomic structure for calculation. **(b)** XRD patterns obtained experimentally at each delay time. **(c)** XRD patterns at 0–10% random displacement of the atomic structure.

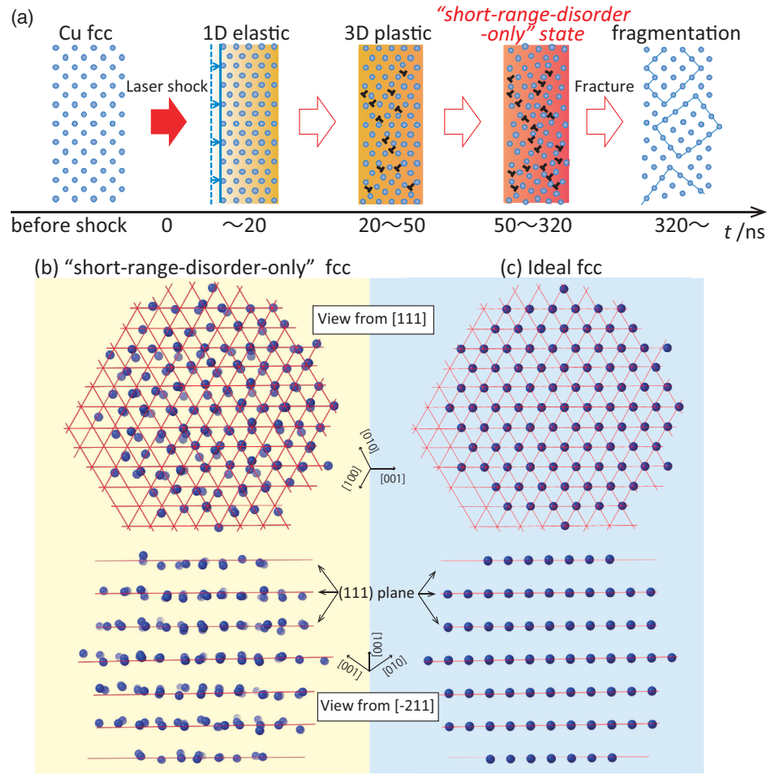

Figure 2: (a) Structural changes in copper during fracture. Conceptual diagram from laser irradiation to fracture and particulation, and atomic structure of the short-range-disorder-only state **(b)** and ideal fcc structure **(c)** viewed from the [111] and [-211] directions, respectively.

Figure 2 [3] shows a conceptual diagram of the process from laser irradiation to fracture and fragmentation of copper and the atomic structure of the "short-range-disorder-only" state. Comparing the experimental and calculated XAFS spectra, the spectrum at 317 ns after laser irradiation is in good agreement with that at 10% displacement, suggesting that only about 10% local displacement occurs at 317 ns, as shown in **Fig. 2(b)**. These results indicate that copper is in a locally heterogeneously disordered but LRO-preserving state (defined as a "short-range-disorder-only" state) after 117 ns.

During plastic deformation, locally inhomogeneous and disordered states occur on planes with low stacking fault energy, such as {111} and {100} planes, and are accelerated by twin formation and slip of high-density dislocations caused by deformation with high strain rates (10^6 s^{-1}) [1, 2]. Then, high-density dislocations form and entangle (tangling), resulting in a highly inhomogeneous strain field. This may be the cause of the "short-range-disorder-only" state that occurs just before the moment of fracture. Based on the above, we conclude that laser-induced fracture of copper proceeds according to the process shown in **Fig. 2(a)**. "Short-range-disorder-only" states in small areas, such as around the crack tip, may be the origin of fracture.

The results obtained in this study provide basic information on fracture trigger sites necessary for designing safety margins of materials and predicting the lifetime of metals. With respect to metal fracture, if the formation of this "short-range-disorder-only" state can be controlled, it will be possible to suppress the number of trigger sites.

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BEAMLINES

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