How to make materials more resistant to extreme deformation

Understanding of the fracture phenomena of a material under extreme conditions of pressure and/or temperature is crucial for a wide variety of scientific fields ranging from applied science and technological developments to fundamental science such as laser-matter interactions and geology. This universal process is particularly important for the development of new materials. Indeed, the properties related to the fracture of materials depend on the way forces are applied to materials as the properties are difficult to define physically. Such properties include the bulk modulus, young's modulus, and spall strength. A method of directly estimating spall pressure may facilitate the efficient evaluation of the spall property to explore novel materials. As an example, there is a large amount of debris around the Earth traveling at an average velocity of ~10 km/s and can hit spacecraft and satellites. If one can test and develop new materials that have different behaviors of dynamic fracture, one can make them more robust or with specific properties (e.g., void size). We have been attempting to bridge the gap between the fundamental study of dynamic fracture and the needs of engineers in materials design, system certification, and manufacturing as discussed in [1].

Several experimental techniques have been developed over the last few decades to study the dynamical damage of a material using macroscopic information, such as the evolution of the free surface velocity and/or information obtained from postmortem examination of the sample. However, a gap exists between the information retrieved at the macroscopic scale from experiments and that obtained from large-scale simulations performed at the atomic scale. In Ref. 2, a new experimental technique is presented, which allows the direct ultrafast real-time monitoring of dynamic fracture (spallation) at the atomic scale with picosecond time resolution. This is achieved in coupling an optical high-power laser (I ~2.5×10^{12} W·cm^{-2}), which generates a shock wave inside the sample (5-μm-thick polycrystalline tantalum), with an X-ray beam (10 keV photon energy) used as a probe. The experimental setup is displayed in Fig. 1 and the experiment has been performed at SACLA **BL3**.

Experimental results are presented in Fig. 2. We were able to directly measure an extension of the tantalum lattice of ~8 to 10% just before fracture occurred at an ultrahigh strain rate of ~2×10^{8}-3.5×10^{8} s^{-1} using X-ray diffraction. The spall strength has also been determined to be approximately –16.8 GPa. These results have been directly compared with large-scale molecular dynamics simulations and are in good agreement with simulated data (see Fig. 3). This not only paves the way toward the direct measurement of the spall strength of materials as a function of strain rate but also highlights the usefulness of these facilities for investigating various physical problems such as high-speed crack dynamics, uncommon stress-induced solid-solid phase transitions, and so forth.

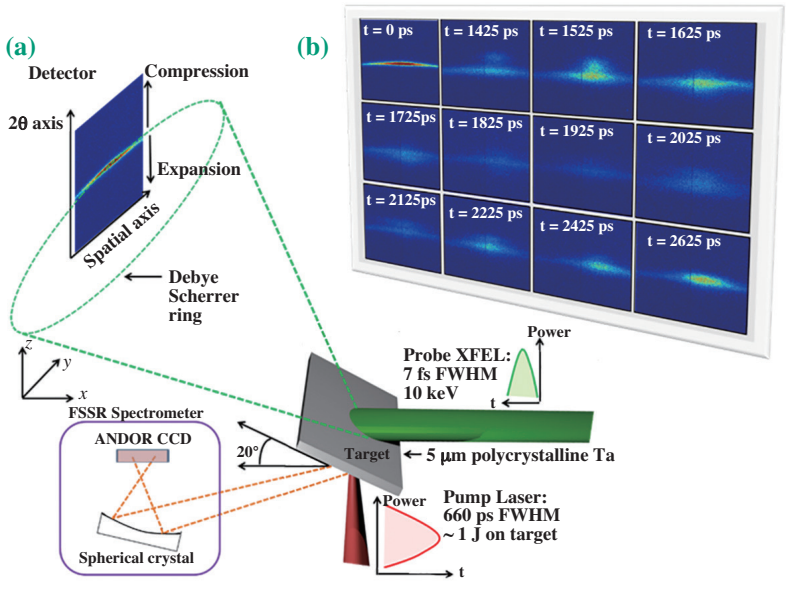

Fig. 1. Pump-probe experiment at SACLA BL3. **(a)** Experimental configuration. **(b)** Experimental results.

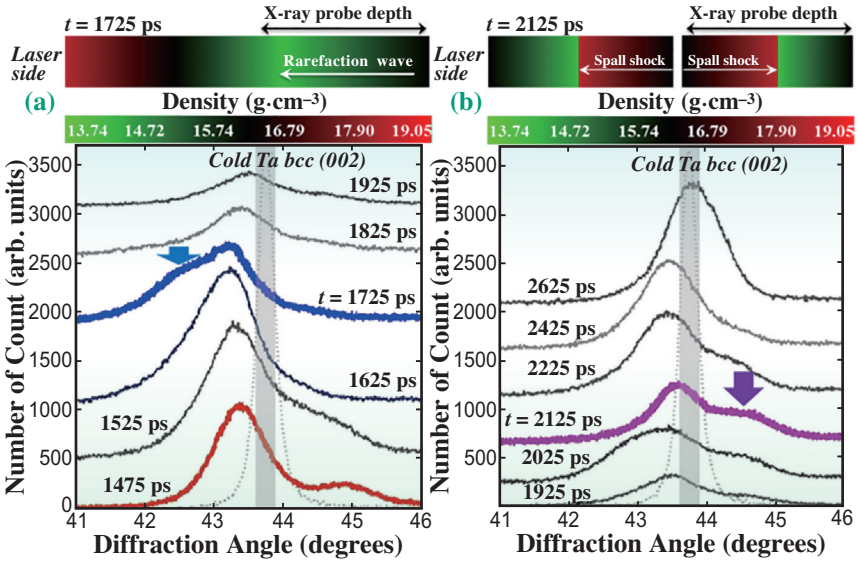

Fig. 2. Experimental profiles of stretching and postspallation compression in a Ta sample. **(a)** Observed stretching (blue curve) of the (002) plane of Ta in the experiment. **(b)** Observed compression wave (purple curve) due to the relaxation of tension after spallation.

As a conclusion, it is interesting to note that the repetition rate of the SACLA platform is non-negligible. This means that it is possible, during one experimental campaign, to test many different materials. This makes it easy to investigate the atomic structures of new materials and select those having the desired macroscopic properties over a wide range of strain rates and deformations. Then, in the next cycle of development, the obtained knowledge about specific relationships between these mechanical properties and atomic structures can be used in the design of the next generation of materials. In this way, XFEL facilities may accelerate the development of new materials by bridging the gap in the understanding of the relationships between atomic structures and material properties.

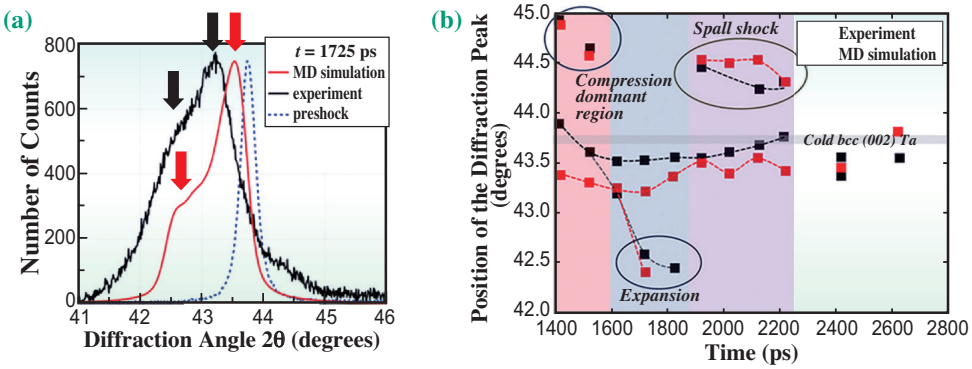

Fig. 3. Comparison between experimental results and those obtained in large-scale atomistic simulation. **(a)** Direct comparison between the diffraction signal obtained in the experiment (black) and simulation (red). **(b)** Dynamical comparison of the position of the peak in the experiment and simulation.

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