Ultrafast probing of the atomic structure of supercooled liquid metals

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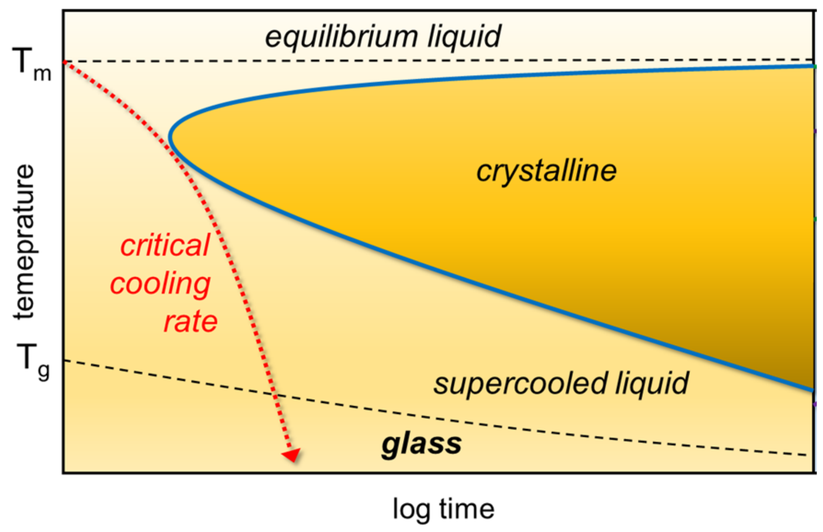
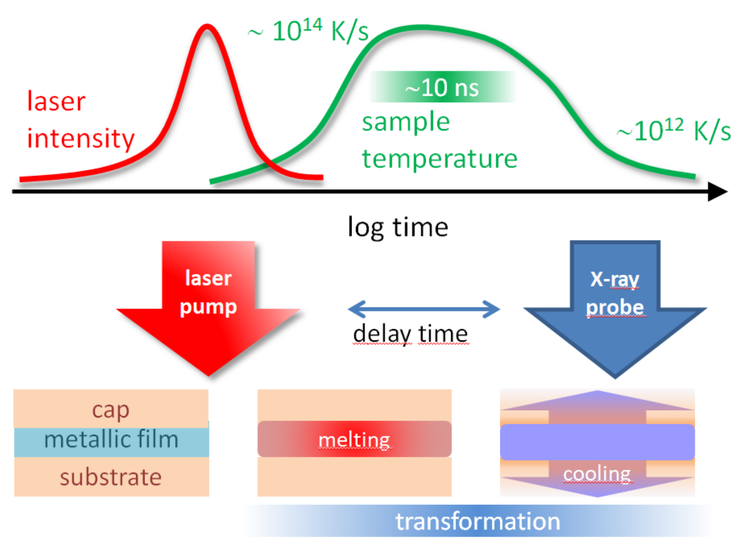
Research objective: Glasses are particular materials that lack the periodic atomic arrangement characteristic for crystals. While glasses are amorphous which means that their atomic order resembles the frozen structure of a liquid, they are mechanically rigid and macroscopically act like solids. The usual route to make a glass is supercooling i.e. quenching a viscous liquid from above melting point down to so called glass transition. Metals are typically poor glass-formers as compared to oxides and polymers. The intrinsic reluctance of liquid metals to form glassy phase on quenching is related to exceptionally fast atomic dynamics below the melting point, leading to crystallization. Due to this time-scale limitation, following structural phase transitions of metals in the high temperature regime is a major challenge. It thus follows that the fundamental mechanisms underlying the formation and stability of metallic glasses remain essentially unknown. Here we propose an experimental approach to overcome this limitation and to trace the structural pathway of highly unstable metallic melts to the highest accessible state of supercoolings.

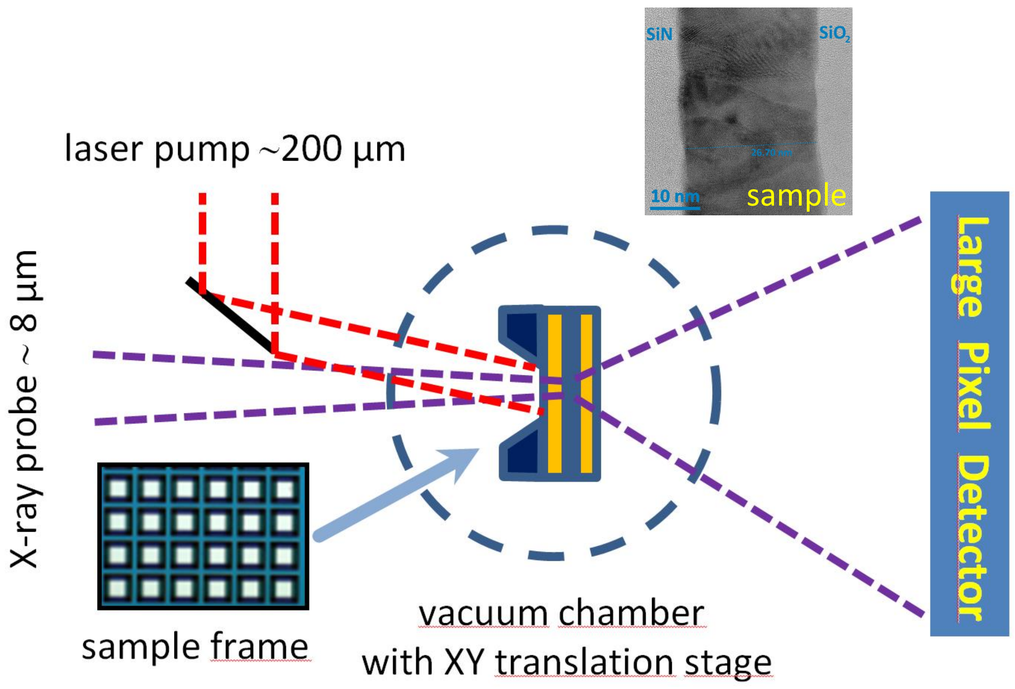
Time-Temperature-Transformation diagram



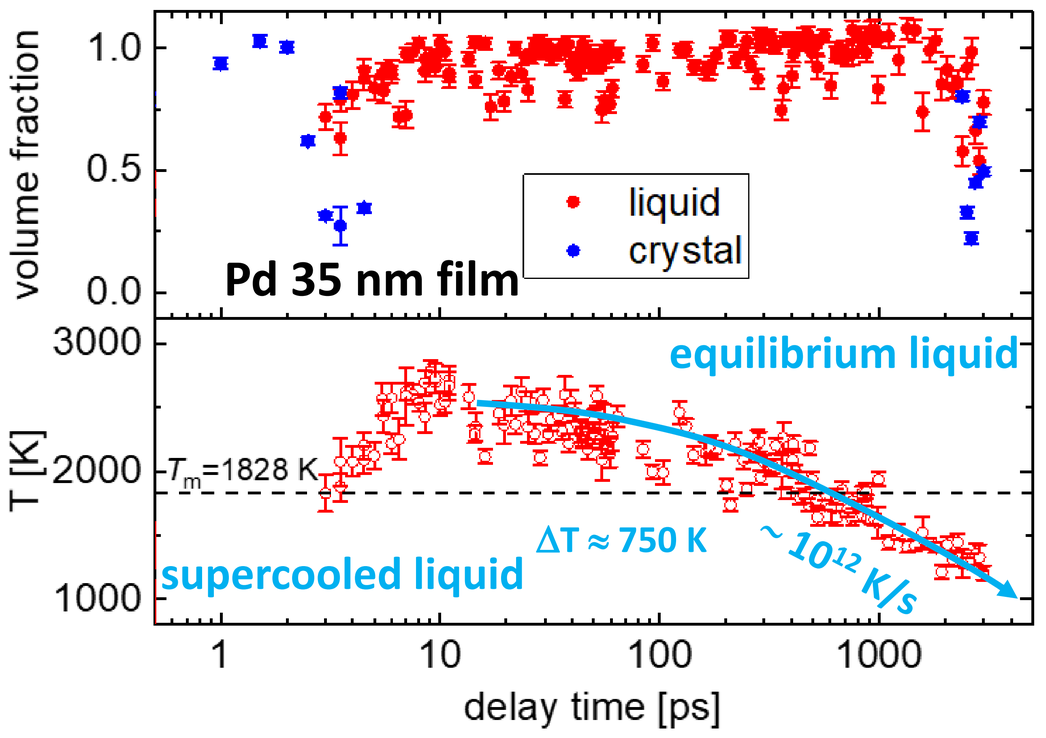
Ultrafast laser quenching



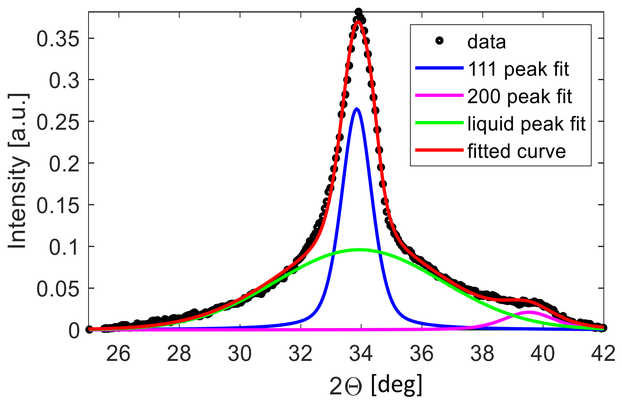
Experimental setup @ FXE station of EuXFEL



Experimental results

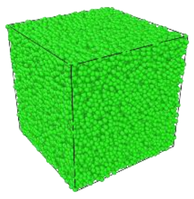


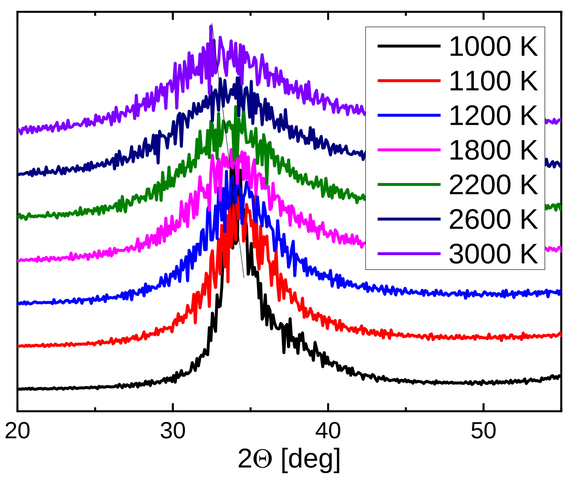
X-ray diffraction data reduction



Molecular dynamics simulations of liquid

- LAMMPS code.
- system: 32 000 of atoms, orthogonal simulation box with periodic boundary conditions, NPT ensemble
- Sheng's EAM potential for Pd
- time step: $\Delta t=10^{-15}$ s
- system annealed @ 3000 K and quenched to 300 K @ 10^{11} K/s
- quenching time: 27 ns
- simulation box edge length ~ 8 nm





Acknowledgments: This work was supported by National Science Centre, Poland, grant agreement No 2017/27/B/ST3/02860.

Conclusions: the atomic structure of deeply supercooled liquid metals was probed by XRD at unprecedented quench rates of 10^{11}-10^{12} K/s allowing direct comparison of the experimental data with predictions of Molecular Dynamics simulations which are intrinsically restricted to extremely fast cooling rates.