

**Experiment title:**

The role of local atomic ordering for the rejuvenation effect in metallic glasses

Experiment number:**HC-3438**

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Report:

A simple thermal treatment is expected to induce a rejuvenation effect in the Gd₆₅Co₃₅ metallic glass, which shows a prominent peak in the β -relaxation, indicating a large structural inhomogeneity in this metallic glass [1, 2]. To discuss the relation between the structural inhomogeneity and thermal relaxation by the repeated temperature changes with the viewpoint of partial structures, we have carried out anomalous x-ray scattering (AXS) experiments to clarify the short- and intermediate-range atomic orders (SRO and IRO) of the as-quenched and thermally treated Gd₆₅Co₃₅ metallic glasses.

Recently, an important research focus is the rejuvenation behavior (i.e. the relaxation to a higher energy state) in metallic glasses. Such an effect can have a pronounced and favorable impact on the plasticity of the glass. The rejuvenation can be induced by repeated thermal changes [1]. According to Ketov et al. [1], there would be distributions of thermal expansion coefficients if a glass is inhomogeneous. In such a glass, shear forces are induced between the parts with large and small volume changes by repeated temperature changes, and there a rejuvenation happens. Therefore, it is suggested that the larger the inhomogeneity is in a glass, the more prominent the rejuvenation is. The validity of the above logic is currently an important subject of discussion.

However, it is impossible to understand the actual structural differences without further information on the partial correlations. The most powerful tool for this purpose is AXS [3,4], especially since the inhomogeneities in the glass are expected to show on SRO and IRO length scales, which AXS can probe simultaneously.

The $\text{Gd}_{65}\text{Co}_{35}$ metallic glass sample was manufactured at Tohoku University, Japan, by splat-quenching from a molten mixture under high-purity Ar atmosphere. A part of the sample was treated by repeated temperature changes by several ten times between room- and liquid N_2 temperatures, which cause a rejuvenation effect. We conducted the AXS experiments close to the K edges of Gd and Co. The experimentally obtained structure factors of the as-quenched and the rejuvenated (thermally treated) sample are displayed in Fig. 1 and Fig. 2. The largest changes are found for the structure factor related to Co, while Gd shows similar features in both samples.

The experimental data were subsequently analyzed by reverse Monte Carlo (RMC) modeling [5]. The resulting partial pair correlation functions are illustrated in Fig. 3. We find that the short-range order is nearly identical in both glasses and next-neighboring peaks are very similar. The interatomic distances are in good agreement with predictions from *ab-initio* calculations on Gd-Co alloys [6]. The differences in the samples are mainly related to the Gd-Co interaction on the intermediate-range level for distances larger than 3 \AA , as indicated by the arrows in Fig. 3. These results demonstrate the special advantage of the AXS technique to probe the IRO for the structural characterization of metallic glasses.

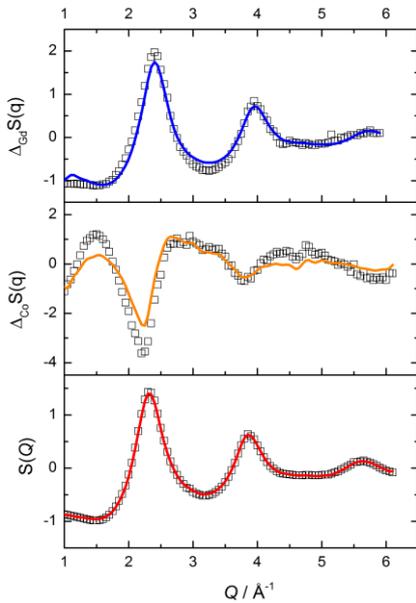


Fig. 1: Experimentally determined $\Delta_k S(Q)$ functions (squares) and RMC fits (lines) of the **as-quenched** sample.

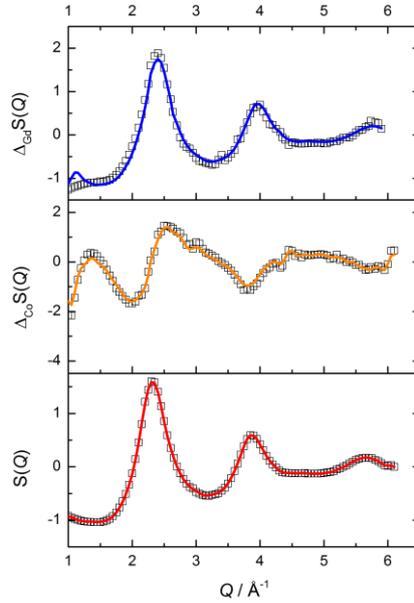


Fig. 2: Experimentally determined $\Delta_k S(Q)$ functions (squares) and RMC fits (lines) of the **rejuvenated** sample.

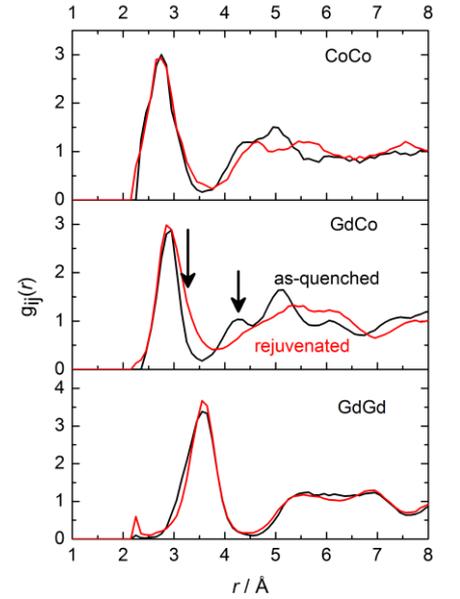


Fig. 3: Partial pair correlation functions obtained from the RMC models.

References

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