Atomic Scale Insight Into The Physical Mechanism Of Aging Process Of Amorphous Alloys

Overview

Amorphous alloys, also known as metallic glass is a solid metallic alloy material with a disordered arrangement of atoms and also non-crystalline with a glass-like structure. It possess unique physical and magnetic properties that combine strength and hardness like metal with toughness and ductility like plastic at room temperature. Amorphous metals are technically glasses, but they are much tougher and less brittle. And unlike common regular glass, amorphous metals display a high degree of electrical conductivity. Therefore, they have been applied in different areas including high efficiency transformers, high frequency transformers and anti-theft tags. Amorphous metals are synthesized by rapidly cooling. It caused the alloy to cool too fast to form a crystalline structure thus metal was locked into a glassy state. This project is focused on the physical mechanism of aging process and relaxation processes. Physical aging can be explored by observing at the temporal evolution of a given material, keep changing other external parameters, such as the temperature and the pressure of the system.

Amorphous alloy

In the case of structural glasses, temperature is often the key parameter that brings the system in the arrested state, by cooling a liquid glass-former fast enough to avoid nucleation and crystal growth. During this process, the viscosity of the system increases dramatically by almost ten orders of magnitude within a narrow temperature range until the material is unable to follow the temperature changes and vitrifies into athermodynamically unstable glassy state. Similar behavior is also observed by increasing the packing fraction in a colloidal suspension, or by applying an external stress in a granular media.

To produce amorphous alloy, there are several ways with different procedures, all of which are complex and require specialized equipment. For instance, mechanical alloying, extremely rapid-cooling, vapor deposition and plasma processing. Furthermore, there are some method amorphize material without passing through the liquid state. It is called solid-state reaction including irradiation, hydrogen-assisted amorphization, interdiffusion of elemental metals, pressure-induced vitrification, and mechanical deformation.

Physical aging

When metal is supercooled below temperature Tg (glass transition temperature), the system will falls out of equilibrium and get to a metastable state through different states toward the corresponding supercooled equilibrium liquid phase. Metallic glasses feature irreversible processes like rejuvenation and memory effects, associated with the existence of a variety of metastable states. Those different metastable glassy states can be experimented with different annealing procedures and cooling rates. Increase the viscosity with decrease of temperature to approach the glass transition temperature (Tg). The glassy state is reached when the system becomes too viscous to follow the temperature changes, and falls out of equilibrium at Tg. The arrow shows the direction of viscosity evolution during the physical aging.

Thus every physical properties of the system depends on the applied experimental protocol and evolve over time due to ongoing relaxation processes which makes the development of a theory for metallic glasses and even a comparison between different experimental results not always possible. This phenomenon, known as physical aging, can produce unnecessary technical deficiencies, because it will adversely affects the service lifetime of glassy materials during operation.

Physical aging in macroscopic insight

Macroscopically, measurable quantities like viscosity, volume and elastic constants are always the subject we want to studies. We investigate those quantities evolve with Tw (waiting time), which depends on the previous thermal history and which can be accurately described by stretched exponential functions. Similar results have been reported in studies of aging effect on the high frequency tail strength of the dielectric spectra All these works provide information on the equilibration toward the supercooled equilibrium liquid phase.

Microscopic details on the aging dynamics in the glassy state can be obtained by studying the temporal evolution of the structural relaxation time, ?, which represents the time necessary for the system to rearrange its structure from a perturbed system into equilibrium. For example, we can measure the value by monitoring its long-term decay of the intermediate scattering function (q, t), on a length scale 2?/q, with the wave-vector q corresponding to the mean inter particle distance. The intermediate scattering function is related to the density-density correlation function and contains all the information on the relaxation dynamics in the system on a length scale determined by q.

Relaxation Process

Amorphous alloys in physical aging

To study relaxation, metallic glasses would be an undeniable choice, because aging can be fast and lead even to ductile-to-brittle transition and crystallization. Both metallic glasses and the melts from which they are formed reveal many structural similarities, which can be readily gleaned from atomic-level diffraction studies. Moreover, the issues of atomic mobility and diffusion in the glassy state, and also relationship with the aging process, we can observe it by focus on the dynamical evolution of the melt as it condenses into an amorphous solid after cooling through the glass transition. Atomic transport in viscous metallic melts is governed by complex and highly collective relaxation dynamics, mainly caused by fluctuations in density and composition, driven by both thermal energy and chemical potential gradients. They strongly influence the long-term self-diffusion of atoms, as well as macroscopic thermophysical properties such as density, shear viscosity and surface tension. However, studying these processes in the necessary details requires a microscopic framework which explains the spatiotemporal behavior of the atoms in the melt. Static and dynamic correlation functions have traditionally been used to obtain statistical insight into the position and motion of particles.

Microscopic operator in relaxation dynamics

Following the formalism of van Hove, the total time dependent pair distribution function (PDF) G(r, t) of a classical liquid can be split into two parts: The first refers to the self-part of G(r, t) and describes the correlation of the positions of a single, tagged particle at different times, while the second correlates pairs of distinct particles and is aptly referred to as the distinct, or collective, part of G(r, t). These functions are usually hidden in reciprocal space, and must first be unraveled via Fourier transforms of data obtained using advanced scattering techniques as those available in large scale facilities such as synchrotrons and neutron sources. Intermediate scattering function (ISF) is a convenient descriptor of atomic motion accessible in various scattering techniques employing laser light, neutrons, x rays, and even electrons, described here in a normalized form.

As it shown from the definition in equation, the temporal evolution of these structural rearrangements is captured by the ISF describing either self- or pair-correlations at different wave numbers q. Therefore, the term‘structural relaxation’will be refer to the microscopic processes underlying the decay behavior of the ISF in metallic melts and glasses. In the sub-picosecond regime, the dynamics is related to the free motion of the atoms and to their collisions and results in a fast decay of the ISF illustrating different relaxation processes in metallic melts from its initial value of 1.

?-relaxation

Generally, for simple metallic liquids comprising single component systems or melts with low atomic packing fractions, atomic transport is dominated by hard-sphere-like binary collisions and the ISF decays to 0 within only a few picoseconds. The functional form of this so-called ?-relaxation is usually well described by a single Debye process, resulting in a simple exponential decay with a characteristic structural relaxation time??. Considering the self-part of the ISF, for example, a simple exponential decay is the result of a diffusion pattern that occurs in the long wavelength limit q ? 0, which is expected from the predictions of fluid dynamics theory. And it can be detected experimentally by using incoherent quasi-elastic neutron scattering (QENS). Noted that the QENS signal is weighted by the interactions of neutrons and atomic nuclei. Therefore it is a selective technique because different nuclei have different neutron scattering cross sections.

Kohlrausch–Williams–Watts expression is employed to describe the long-time decay of the ISF corresponding to the ?-relaxation.

Secondary relaxations

Schedule of the dissertation. Dates Schedule September to early October Literature review to understand the project Mid October to early November Investigate the synthesized zirconia ceramics under laser treatments and hydrothermal Early November to December Investigate the synthesized zirconia ceramics under mechanical loads.