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ScienceDirect
Scripta Materialia 60 (2009) 273–276
Scripta MATERIALIA
www.elsevier.com/locate/scriptamat

Thermomechanical properties of gold nanowires supported on a flexible substrate

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Received 8 May 2008; revised 19 August 2008; accepted 29 August 2008
Available online 5 November 2008

Diffusion-controlled deformation mechanisms may become relevant for nanocrystalline and nanostructured materials at room temperature. In this paper, the stress–strain behavior of gold nanowires 40 nm wide, 20 nm high and 1 mm long on a flexible substrate was investigated in the temperature range of 173–393 K. For decreasing temperatures, the yield strength and the fracture resistance increase. Both can be qualitatively explained by diffusion-driven deformation. The activation energy at room temperature indicates diffusion on (1 1 1) surfaces.

Keywords: Yield Strength; Diffusional creep; Temperature; Gold nanolines

The yield stress of face-centered cubic (fcc) bulk materials is usually independent of temperature below a homologous temperature of 0.5, which is well established to be due to dislocation glide. Above this critical homologous temperature, pinned dislocations can climb and overcome their obstacles by thermal activation (cf. Fig. 4.18 in Ref. [1]). For nanocrystalline fcc materials, diffusion-controlled deformation mechanisms such as grain-boundary sliding and Coble creep may become significant even at room temperature (RT) since the diffusion paths are very short. Masumura et al. [2] proposed that the experimentally observed inverse Hall–Petch relation for grain sizes below 20 nm could be explained by Coble creep. Gruber et al. [3] reported a strong temperature dependence of the yield strength of homogeneous gold thin films in the thickness range of 80–500 nm on flexible substrates by a grain-boundary diffusion mechanism. On the other hand, Lin et al. [4] concluded from their strain-rate-dependent experiments on pure gold and vanadium-doped gold thin films ($T \sim 0.35$–$0.5T_m$) that thermally activated dislocation motion could be the only relevant inelastic mechanism. Liu and Chao [5] interpreted temperature-dependent strain rate effects, yield strengths and ductility in doped micrometer gold-bonding wires as diffusional flow. Chasiotis et al. [6] performed tensile testing of freestanding gold thin films in the thickness range of 500–2200 nm (grain size 70–120 nm) and reported a strong strain rate dependence of the yield strength by power law creep at RT. The strong strain rate dependency is consistent with findings of Emery and Povirk [7] on freestanding and fine-grained gold films with grain sizes of several hundred nanometers. From molecular dynamics simulations on (1 1 1) oriented gold nanopillars under compression Rabkin and Srolovitz [8] found yield strengths with either linear or parabolic relationships on the temperature (in the range 0–150 K). They suggested the glide of Shockley partials, which are nucleated at the surface of the pillars, to be the dominant deformation mechanism [8,9]. For bulk nanocrystalline Cu (30 nm grain size), Cai et al. [10] report Coble creep at homologous temperatures of about 0.2. Surprisingly, Li et al. [11] observed a similar behavior on more coarsely grained material.

This paper focuses on the temperature dependence of the yield strength and the onset of cracking of gold nanowires on flexible polyimide substrate. In contrast to the studies described above, these samples are nanocrystalline (20–30 nm grain size) as well as nanostruc-

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doi:10.1016/j.scriptamat.2008.08.046

tured (20 nm high, 40 nm wide and 1 mm long), which is expected to result in slightly different deformation mechanisms.

Parallel line arrays of gold were produced by a combination of extreme ultraviolet interference lithography and a lift-off process using the XIL beamline of the Swiss Light Source (SLS) [12]. The parallel line arrays consist of 5000 identical nanowires 40 nm wide, 20 nm high and 1 mm long with a periodicity of 100 nm. Polyimide foil (Kapton™, Du Pont) 125 μm thick was used as a substrate. An improved adhesion of the gold nanowires was achieved by a 2 nm chromium interlayer at the Kapton™/nanowire interface.[1] Details of the procedure are described in Ref. [15].

The nanowires were tensile tested by the $\sin^2(\varphi)$ technique using the powder diffraction stage of the Materials Science beamline at the SLS [16]. Details of the testing procedure are described by Bohm et al. [17] and in the authors' previous work [13,14]. Tuning the energy of the X-rays to the (1 1 1) out-of-plane texture of the gold nanowires ($E = 7.91$ keV) resulted in a strong Debye–Scherrer ring. Its deformation due to externally applied strain was monitored by two second-generation microstrip detectors [18,19] corresponding to the principle axes of the Debye–Scherrer ellipse. The applied strain was measured by tracking optical strain markers close to the parallel line arrays. The proximity of the markers to the nanowire arrays is necessary since the local effective applied strain differs from the applied global strain (which was the same for all samples). This is due to the local control of the temperature T_t of the samples during the tensile tests with a CryoJet (Oxford Instruments) in the range 173–393 K.

Representative results of the $\sin^2(\varphi)$ experiments are shown in Figure 1. In general, the stress–strain behavior of the nanowires follows a linear relationship upon loading and subsequently reaches an upper plateau. Upon unloading, the stress–strain curve shows again a linear relation and finally reaches a lower plateau. The amplitude of the plateaus corresponds to the yield strength of the nanowires and strongly depends on T_t, which is demonstrated in Figure 2. Samples tested at $T_t = \mathrm{RT}$, $T_t = 343$ K and $T_t = 393$ K show a drop in the stress–strain curve for $\varepsilon > 6.7\%$, $\varepsilon > 5.8\%$ and $\varepsilon > 3.2\%$, respectively, indicating the formation of cracks [20] (e.g. vertical arrow at $\varepsilon = 5.8\%$ for sample I in Fig. 1). The corresponding threshold strain ε_c is defined as the onset of cracking.[2] In contrast, samples tested at $T_t = 173$ K and $T_t = 223$ K do not show any indications of crack formation. An overview on the experimental findings and parameters is given in Table 1.

The strong temperature dependence of the yield strength is unusual for bulk fcc materials such as gold [1]. For analysis, a diffusional mechanism is chosen because of (i) the presence of free surfaces, (ii) the extremely small grain size of 20–30 nm (short diffusion paths and the absence of stored dislocations) and (iii) the very low strain rates applied (cf. Table 1). According to Gruber et al. [3], a general diffusional creep equation is assumed:

$$\dot{\sigma} = E \cdot (\dot{\varepsilon}_{\mathrm{ext}} - \dot{\varepsilon}_{\mathrm{p}}) = E \cdot (\dot{\varepsilon}_{ext} - C \cdot \sigma), \tag{1}$$

where E is Young's modulus, $\dot{\varepsilon}_{\mathrm{ext}}$ is the constant external applied strain rate, $\dot{\varepsilon}_{\mathrm{p}}$ is the relaxation strain rate due to diffusion controlled plastic deformation and C is a factor which is characteristic for the dominant diffusion mechanism. With the boundary condition $\sigma(\varepsilon = 0) = \sigma_0$, Eq. (1) can be solved by:

$$\begin{aligned}\sigma(\varepsilon) &= \frac{\dot{\varepsilon}_{\mathrm{ext}}}{C} - \left(\frac{\dot{\varepsilon}_{\mathrm{ext}}}{C} - \sigma_0\right) \cdot \exp\left(-E\frac{C}{\dot{\varepsilon}_{\mathrm{ext}}}\varepsilon\right) \\ &= a + b \cdot \exp(-c \cdot \varepsilon).\end{aligned} \tag{2}$$

The stress–strain curves can be fitted well by Eq. (2) for $\varepsilon < \varepsilon_c$, which is shown in Figure 3 exemplarily for samples B, F and K. The corresponding fitting constants a, b and c are listed in Table 1. The characteristic factor C for the diffusion mechanism generally shows a temperature dependency:

$$C \propto \frac{1}{k_B T} \exp\left(-\frac{E_{\mathrm{act}}}{k_B T}\right), \tag{3}$$

where k_B is Boltzmann's constant, T is the absolute temperature and E_{act} is the thermal activation energy. The activation energy is obtained by an Arrhenius plot of

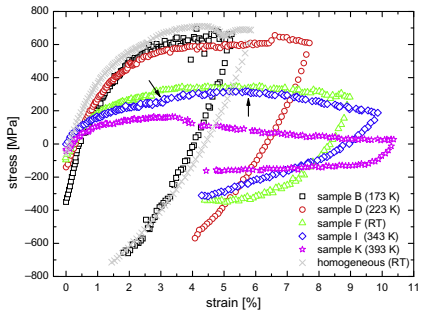

Figure 1. Representative stress–strain curves (loading direction) of gold nanowires about 40 nm wide, 20 nm high and 1 mm long for different testing temperatures T_t. The vertical arrow marks the point of doubling the strain rate and the sloping arrow marks the onset of cracking for sample I (RT).

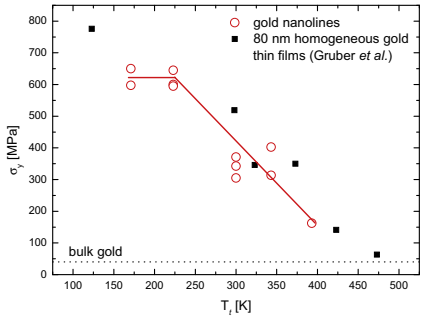

Figure 2. Yield strength of the nanowires as a function of the testing temperature. The yield strength clearly shows strong temperature dependence: the higher the testing temperature, the lower the yield strength. For comparison, the yield strengths of homogeneous 80 nm gold thin films (without an adhesive interlayer) are also shown [3].

[1] Note that in contrast to our previous work [13,14] the adhesive chromium interlayer between the polyimide substrate and the gold nanowires was changed from homogeneous to line space patterned just below the gold lines.

[2] The onset of cracking ε_c was obtained by the intersection of $d\sigma/d\varepsilon$ and the abscissa (where "statistical" intersections are not considered). The corresponding accuracy was estimated to be ±0.25%.