Low Temperature Measurements of Lattice Parameter of Microcrystalline Gold

W. Paszkowicz, R. Minikayev, P. Piszora[1], M. Knapp[2] and C. Bähtz[3]

Institute of Physics, P.A.S., Al. Lotników 32/46, PL-02668 Warsaw, Poland (paszk@ifpan.edu.pl)
[1]Adam Mickiewicz University, Faculty of Chemistry, ul. Grunwaldzka 6, PL-60780 Pozna , Poland
[2]Institute for Materials Science, Darmstadt University of Technology,
Petersenstr. 23, D-64287 Darmstadt, Germany
[3]Hasylab at DESY, Notkestr. 85, Hamburg, Germany

Gold is one of important technological materials. Its properties like high chemical inertness, electrical conductivity, malleability, ductility, non-corrosiveness, are widely exploited in technology. It is not possible to enumerate all applications of gold. This noble metal is widely used in catalysis, bionanotechnology, biophotonics. Gold nanoparticles are of particular interest, especially in molecular recognition. Gold can be considered as a quantum-dot material applicable to light emitting sources in nanoscale optoelectronics and biological labels. A gold buffer layer has been found to promote, at stress conditions, a HP structure of deposited CdSe quantum dots. Au is known to form single rows of atoms (quantum wires) on Si(557) surface. Au dots on a Si substrate have been proposed as efficient working structure of solar cells. Moreover, gold has some applications in X-ray diffraction studies. Namely, i) it is a standard used as calibrant in high-pressure diffraction studies, see *e.g.* Refs [1-3], ii) temperature calibration with Au has been proposed (*e.g.* in Ref. [4]) and used (*e.g.* in Ref. [5]) to high-temperature diffraction purposes. Quality of temperature calibration depends on the precision of data of lattice-parameter temperature variation. Extending of the method to low temperature requires knowledge of a high-precision experimental $a(T)$ run.

The purpose of the present study was to determine the lattice parameter for polycrystalline gold in a low-temperature range. The low temperature X–ray diffraction studies were carried out with a powder diffractometer [6] installed at the Hasylab B2 bending–magnet beamline, using the Debye–Scherrer geometry and a wavelength of 0.500 Å. The beam spot size was 1×15 mm^2. An image plate counter (OBI) and alternatively a NaI scintillation counter, were applied for the data collection in low-resolution and high-resolution modes, respectively, in the 2θ ranges of 60° and 3.53°. A closed–circuit He–cryostat ensured the temperature stability and accuracy better than 0.5 K. The data were calibrated using an internal diamond standard. This kind of calibration described in Ref. [8] is suitable for removing of errors such as those due to wavelength fluctuations. A related methodology was successfully applied earlier to spinel type silicon nitride [6]. A mixture of commercial micrometer-size gold (highly diluted) and diamond powders (both from Aldrich) was loaded into a thin–wall 0.8 mm diameter glass capillary (Hilgenberg). For lattice parameter refinement, the Rietveld method (Fullprof.2k program [7]) was applied.

The lattice parameter for the microcrystalline gold was determined at the temperature range from 15 to 310 K. The a value remains almost constant up to about 30 K, in agreement with the dilatometric results showing a vanishing thermal expansion coefficient in this range [9], and then starts to increase with temperature. Preliminary results of calculation of Au lattice-parameter values determined from the OBI data in the 100-310 K range are presented in Figure 1. Polynomial fitting indicates that the experimental value of the measured lattice parameter at 300 K is 4.07818 Å. The calibration applied in this study is based on the Sato *et al.* [10] scale determined for a pure-diamond single crystal. The expected error in diamond lattice parameter (due to a possible difference in defects and impurities between the scale of single crystal and the powder used) is of the order of $\Delta a/a = 3\times10^{-5}$, *i.e.* it is by about 100 times smaller than the observed variation range for gold (for which the full change in the temperature interval studied is $\Delta a/a = 3.4\times10^{-3}$). Therefore, its possible influence on the $a(T)$ run of gold due to application of single-crystal diamond scale instead of polycrystalline scale can be neglected. The refinement results for the data collected using the NaI counter exhibit a slightly better accuracy than those obtained with the OBI imaging plate.

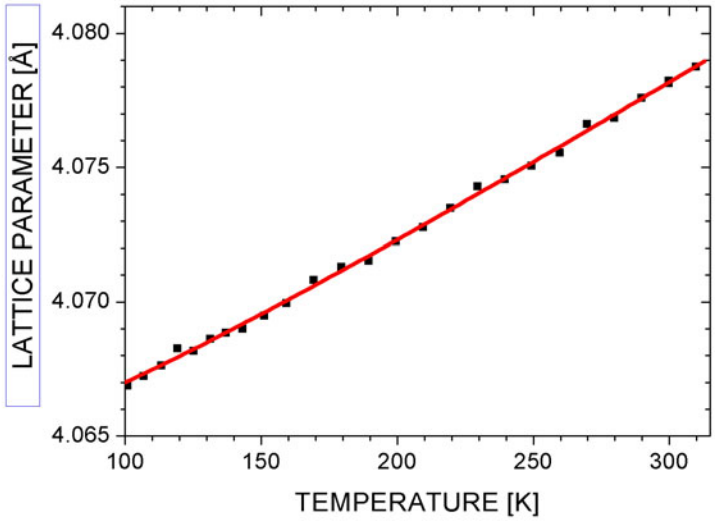

Figure 1: Temperature dependence of the lattice-parameter of gold in the 100-310 K range

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References

[1] Y.W. Fei, H. Li, K. Hirose, W. Minarik, J. Van Orman, C. Sanloup, W. van Westrenen, T. Komabayashi, and K. Funakoshi, Phys. Earth Planet. Interiors 143, 515 (2004)
[2] L.C. Ming, M.H. Manghnani, J. Balogh, S.B. Qadri, E.F. Skelton, and J.C. Jamieson, J. Appl. Phys. 54, 4390 (1983)
[3] S.-H. Shim, T.S. Duffy, and K. Takemura, Earth Planet. Sci. Lett. 203 (2002) 729-739
[4] R.O. Simmons, J. Appl. Phys. 41, 2235 (1970)
[5] K. Fukuda, A. Moriyama, and T. Iwata, J. Solid State Chem. 178, 2144 (2005)
[6] W. Paszkowicz, R. Minikayev, P. Piszora, M. Knapp, C. Bähtz, J.M. Recio, M. Marqués, P. Mori-Sánchez, L. Gerward, and J.Z. Jiang, Phys. Rev. B 69, 52103-1 (2004)
[7] J. Rodriguez-Carvajal, Newslett. IUCr Commission Powd. Diffr. 26 (2001) 12
[8] W. Paszkowicz, M. Knapp, C. Bähtz, R. Minikayev, P. Piszora, J.Z. Jiang, and R. Bacewicz, J. Alloys Compds 382, 107 (2004)
[9] F.C. Nix, and D. MacNatr, Phys. Rev. 60, 597 (1941)
[10] T. Sato, K. Ohashi, T. Sudoh, K. Haruna, and H. Maeta, Phys. Rev. B 65, 092102 (2002)