

# Thin Films and Coatings

## MS.5.P129

### Controlling the orientation-relationship between Ni (111) and sapphire (0001)

Z. Fogarassy<sup>1</sup>, G. Dobrik<sup>2</sup>, L.K. Varga<sup>3</sup>, L. Biró<sup>2</sup>, J. Lábár<sup>1</sup>

<sup>1</sup>MTA TTK MFA, Thin Film Physics Department, Budapest, Hungary

<sup>2</sup>MTA TTK MFA, Nanostructures Department, Budapest, Hungary

<sup>3</sup>Institute for Solid State Physics and Optics, Wigner Research Center for Physics, Budapest, Hungary

labar.janos@mta.ttk.hu

Keywords: Ni, Sapphire, double-positioning

Epitaxial growth of Ni (111) on sapphire (0001) was studied during DC magnetron sputtering in ultrahigh vacuum. Commercial sapphire (0001) single crystal was used as a substrate. During growth the substrate temperature was 300-750°C, and the growth velocity was 0.2 nm/s or 0.5 nm/s for the different samples. In some of case bias was also applied. The orientation relationship was investigated with transmission electron microscopy (TEM).

Our aim was to produce a good quality single crystal nickel (sc-Ni) thin layer, which can serve as an inexpensive substrate for graphene deposition. Earlier investigations reported only that the Ni (111) planes were parallel to the Sapphire (0001) and so to the substrate surface [1] and termed it epitaxial growth, although in-plane orientation was not studied.

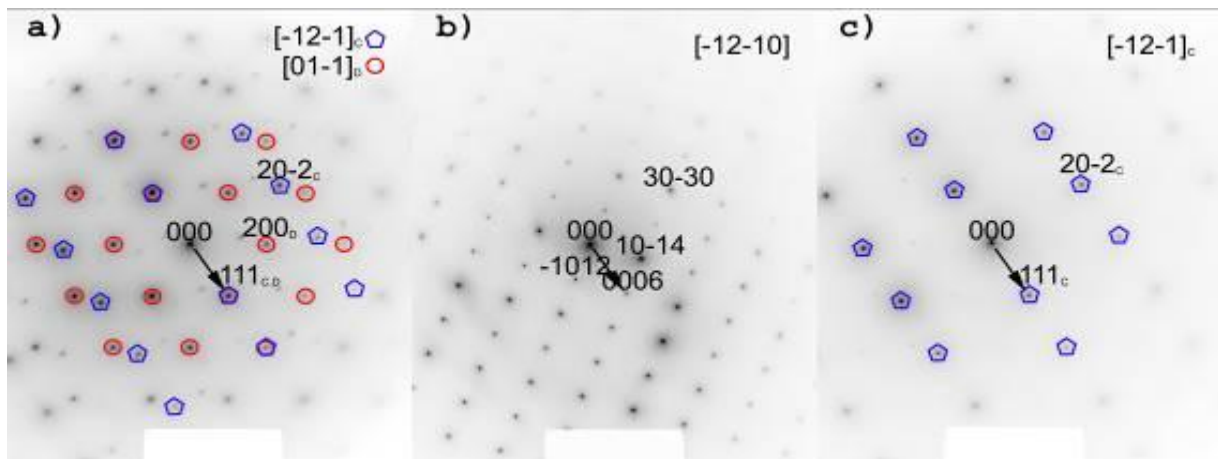
In the present investigation two kinds of epitaxial orientations were detected in the same sample. In both cases the Ni (111) lattice planes were parallel with the Sapphire (0001) lattice planes, but the two different orientations are rotated to each other with 30 degrees around the axis perpendicular to the surface. The sapphire [10-10] is parallel either to the nickel [110] or to the [211]. In the first case the lattice misfit is -9.29 %, which means nickel needs to be compressed to fit to the sapphire and below this orientation will be called the “compressed” orientation. In the second case the misfit is +4.68 %, it will be called the “diluted” orientation. Figure 1.a shows a selected area diffraction pattern from a cross-sectional TEM sample, where both epitaxial orientations are present. The surface normal of the sapphire is marked by the arrows on the diffraction pictures. The sapphire diffraction is shown in Figure 1.b. Figure 1.c shows only the reflections that belong to the “compressed” orientation. Twin boundaries were found in both types of orientations. These twin boundaries are perpendicular or parallel to the surface as it can be seen in Figure 2.

In the sample grown at 550°C temperature with 0.2 nm/s deposition rate, both kinds of orientations were present, but with larger flux (0.5 nm/s) only the “compressed” orientation formed. Using bias, it was possible to produce a Ni layer containing only the “diluted” orientation. In the sample with higher temperature (750°C) and small flux, dominantly the “compressed” orientation appeared.

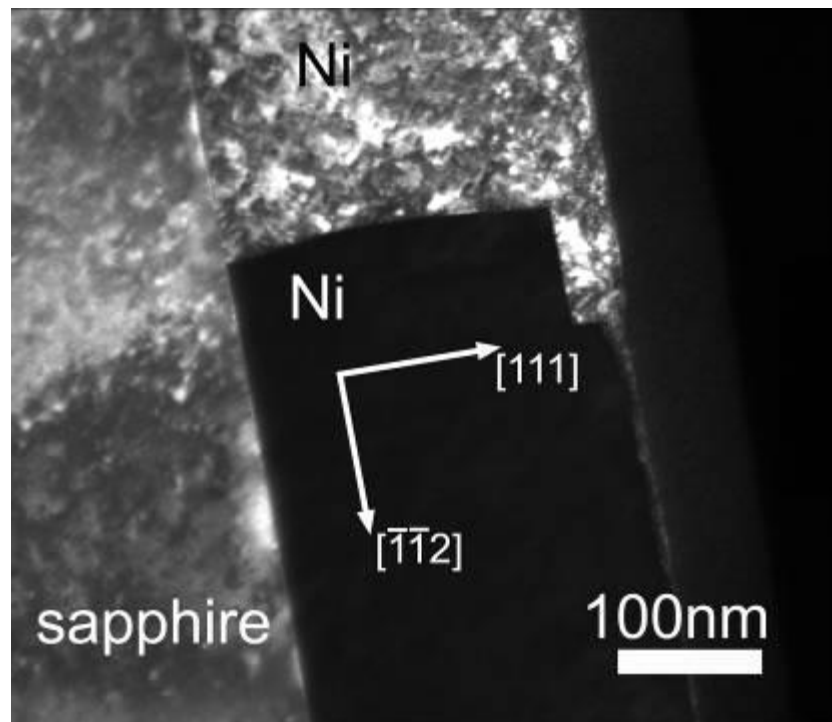
Earlier calculations on non-relaxed structures showed that the “compressed” orientation matches better to the sapphire surface than the “diluted” orientation, although the “diluted” orientation can also exist energetically [2]. However, the “compressed” orientation has a larger misfit than the other one and it stores a larger elastic energy. Our present experimental observations can be explained with the above reasoning. When the nucleus size is small then better adhesion will dominate and “compressed” orientation forms. When the nucleus size is larger, the orientation with the smaller misfit will be energetically more favorable and growth of the “diluted” orientation is preferred.

By controlling the initial nucleation density and the size of nuclei with temperature and deposition rate, it was possible to foster the formation of the pre-selected in-plane orientation of the nickel (epitaxial to the single crystal sapphire (0001) substrate) and to get single crystalline nickel with a single in-plane orientation only. Details are published separately [3].

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2. W. Zhang, J.R. Smith, A.G. Evans; Acta Materialia 50 (2002) 3803–3816.
3. Zs. Fogarassy, G. Dobrik, L.K. Varga, L.P. Biró, J.L Lábár: Growth of Ni layers on single crystal sapphire substrates. Thin Solid Films, submitted for publication.



**Figure 1.** Selected area diffractions taken on a cross-section TEM sample. The direction of the sapphire surface normal is marked by the arrows. Diffraction a) shows a grain boundary area where both the “compressed” and “dilated” orientations are present. The reflections from the “dilated” orientation are marked by the circles, while those from the “compressed” orientations are marked with pentagons. Diffraction b) shows the reflections of the sapphire. Diffraction c) shows the reflections of the “compressed” orientation. The {111} planes coincide for both the “compressed” and the “dilated” orientations and are parallel to the (006) plane of sapphire.



**Figure 2.** Dark field image taken on a cross-section TEM sample. The light (top) and dark (bottom) areas within the Ni layer show the twinned crystallites and the directions of their faceted grain boundary. It can be seen that the grain boundary is formed from facets of {111} and {211} planes, characteristic of the coherent and incoherent twins in fcc materials.