Crystallographic Orientation of Epitaxial Transition Observed for Nb (bcc) on MgO and Cu (fcc) Single-crystals

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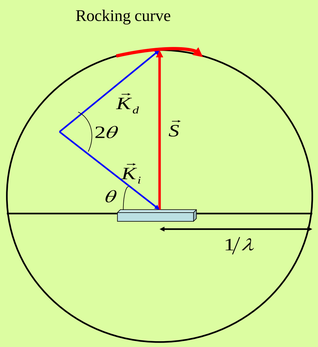
Summary

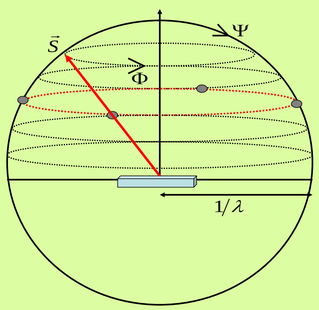
Niobium thin films were grown on (001) MgO single-crystal using a coaxial energetic deposition. The quality of the substrate surface and epitaxial Nb layers were investigated by XRD Bragg-Brentano and pole figure measurements. Depending on growth temperature, in-plane XRD show Kurdjumov-Sachs (KS) as well as Nishiyama-Wassermann (NW) epitaxial relationships for (110) and (001) Nb on (001) MgO. Calculation of the interface energy in rigid lattice models finds one KS and two NW minima. For the NW case the optimal atomic diameter ratio d_{bcc}/d_{fcc}=0.866 and 1.061, whereas for the KS case it is at d_{bcc}/d_{fcc}=0.919. Transitions of this type are usually induced by a change in the lattice parameter ratio resulting from a relaxation process in the early stage of the growth.

X-ray Analysis

X-ray diffraction is one of the most powerful and widely used techniques for accurate characterization of the lattice parameters, mismatch, and thickness of epitaxial materials.



Schematic of scan vector of 2theta-omega scan and rocking curve in reciprocal space

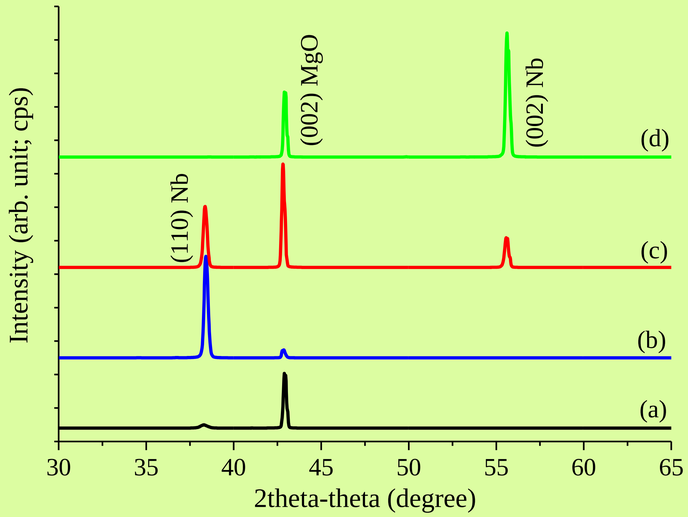


Schematic of scan vector of pole figure measurement in reciprocal space

Sample Information

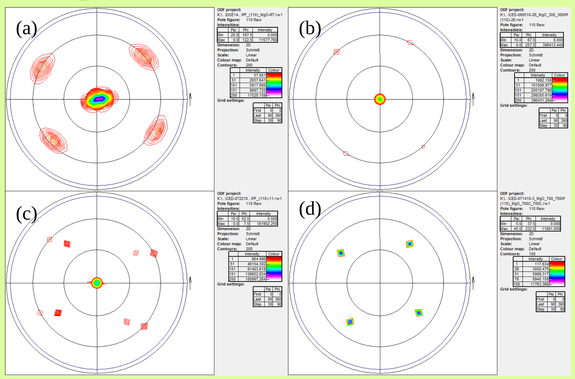
	Ts (°C)	Substrate	RRR	Tc (K)	B-B XRD
DOE146-0702-4	RT/150	(001) MgO	7	9.0	(110) Nb
CED-080510-26	300/300	(001) MgO	48	9.24-9.26	(110) Nb
CED-072210-10	500/500	(001) MgO	181	9.25	(110) & (002) Nb
CED-071410-3	700/700	(001) MgO	316	9.22-9.25	(002) Nb

Out-of-plane XRD



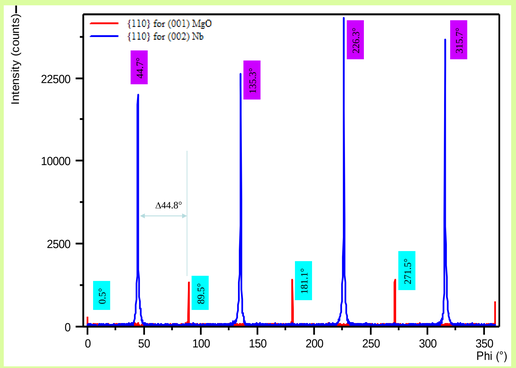
Bragg-Brentano XRD patterns of Nb films on (001) MgO obtained as a function of substrate temperatures of (a) 150°C, (b) 300°C, (c) 500°C, and (d) 700°C.

In-plane (texture) XRD

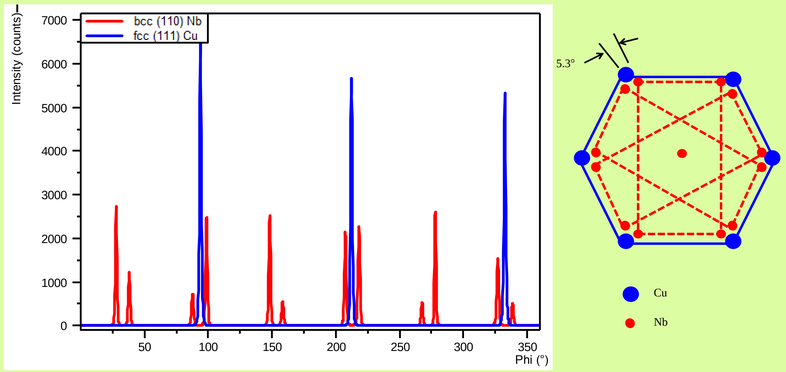


The center spot indicates the grains oriented with (110) planes parallel to the substrate, while four spots at 60° of tilt correspond to diffraction intensities from {110} in-plane texture. The angle between (110) and (100) in cubic materials is 45° that those four peaks emanate from Nb with $(001)_{Nb} \parallel (001)_{MgO}$.

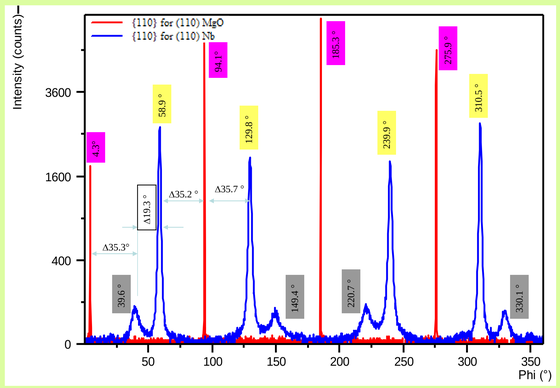
Phi scan {110} for (100) Nb on (100) MgO at Ts=700°C



Phi scan {110} for (110) Nb on (111) Cu at Ts=500°C



Phi scan {110} for (110) Nb on (100) MgO at Ts=300°C



Conclusions

Bragg-Brentano XRD revealed that epitaxial (110) Nb films on MgO substrate were grown under 400°C of deposition temperature and (001) Nb films at higher 600°C, while the diffraction peaks of Nb films were changed from single orientation to a mixed state (110) and (001) plane of 500°C. In-plane XRD (110) and (001) Nb/MgO phi scan with a variety of different NW (Nishiyama-Wasserman) -KS (Kurdjumov-Sachs) states that show the transition independently from substrate temperature. In this state of the transition the NW at orientation θ= 0° one-peak structure is superposed by the two KS peaks appearing at about ±10° relative to the NW direction. For (110) Nb on (111) Cu substrate, optimal ratio is very close to the KS minimum with orientation θ = 5.3°. Clearly, the lattice parameter ratio is an important variable in the epitaxial growth.

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