

ATOMIC SCALE OF NANOLAYER COMPOSITES

A stacking fault is a one or two layer interruption in the stacking sequence of the crystal structure. These interruptions carry a certain stacking fault energy (SFE).

High SFE materials such as Al do not form twins easily. However, researchers have shown that it is possible to form Al layers in twin orientation to each other across polar TiN layers, if these are grown so that both the Al and TiN layers have a {111} surface as their growth front. Al-TiN multilayers were deposited at room temperature on Si substrates using dc magnetron sputtering in the two following different layer thicknesses: Al-9nm/TiN-1nm.

HREM-STEM image I collected by a HAADF detector, showed two Al layers separated by a TiN layer. It was seen that the Al layer is always the one that has a twin orientation with respect to the TiN and Al layers below it. The situation is schematically illustrated in the figure below. Theoretical ab initio calculations based on density functional theory (DFT) revealed that nitrogen termination in the {111} growth plane of the TiN layers greatly favors the growth of twin oriented Al layers on them, thus, being in excellent agreement with experimental observations.

In conclusion, it was shown that in magnetron sputtered Al-TiN multilayers, consecutive Al layers grow in twin orientation with respect to each other when the intervening TiN layers are 1–2 nm thick.

The above HREM experimental data were explored further by means of the ASTAR system that was able to produce orientation / phase maps of the Al-TiN nanolayers revealing clearly the TiN layer of 1 nm thickness. ASTAR orientation maps show clearly the twin orientation relationship between successive Al layers.



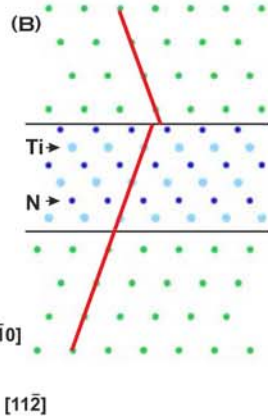
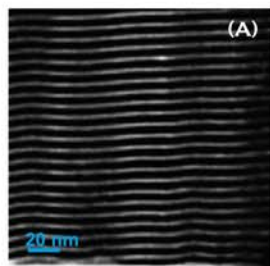
The challenge:

Identify orientation / phase of 1 nm TiN layer in a Al-9nm / TiN-1nm nanolayer composite while TiN and Al differ <5% in cell parameter

Solution:

ASTAR technique coupled with precession electron diffraction

Moreover, these findings suggest a method of introducing nanoscale twins in high SFE materials in general. Since the deposition of Al and TiN layers is used in the formation of diffusion barriers, it is important to investigate and understand these structures at the nanometer length scale and hence to be able to control them.



Crystal Structure

Al: fcc cubic $a = 4.05 \text{ \AA}$
TiN: fcc cubic $a = 4.24 \text{ \AA}$

Experimental Data

TEM type: Jeol 2100 F
Map resolution: 1 nm
Scanned area: 200 x 200 nm

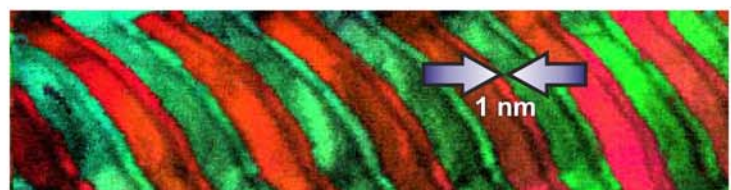
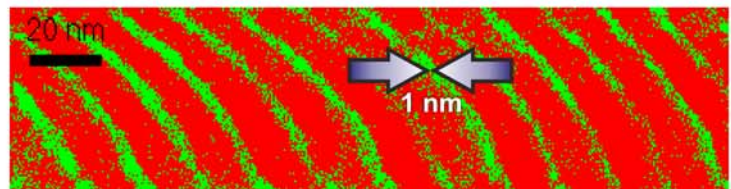
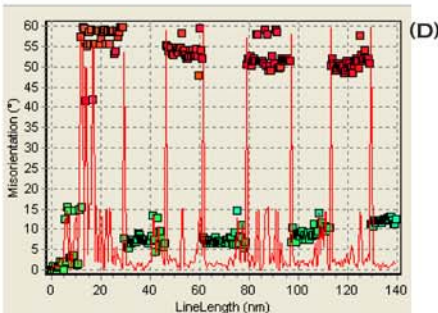


figure 1

(a) HAADF image of Al-9nm/TiN-1nm multilayer system (b) atomic model of the Al-TiN-Al interface (c) ASTAR orientation map where Al layers are shown in red, TiN 1nm layer shown in green (d) line profile of ASTAR orientation map showing twin-related Al layers (E) ASTAR orientation map with 1 nm TiN layers shown as black strips