"On the growth and mechanical properties of non-oxide perovskites and the spontaneous growth of soft metal nanowhiskers"

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Abstract

It has previously been suggested based on *ab initio* calculations that perovskites with the general formula of AB_3X, where *A* and *B* are metals, and *X* is B, C, or N, may exhibit unique mechanical properties such as superior ductility, and hence damage tolerance. In the first part of this thesis, the mechanical behavior of ternary perovskite borides and iron based perovskite nitrides is explored. YPd_3B, Fe_4N, $ZnFe_3N$, and $PdFe_3N$ thin films were synthesized by combinatorial magnetron sputtering, and the mechanical properties thereof were probed by nanoindentation. Generally, the measured elastic moduli were in good agreement with *ab initio* data. The evaluation of the critical shear stress for the onset of plasticity suggests that YPd_3B, Fe_4N, and $PdFe_3N$ can be classified as ductile materials, which is also consistent with the prediction from *ab initio* calculations.

The second part of the work demonstrates a possible application of the combinatorial thin film approach for the fabrication of one-dimensional nanostructured materials. In-Y thin films with a compositional spread were deposited by combinatorial magnetron sputtering. It was found that In-whiskers were extruded spontaneously from the film surface upon exposure to atmosphere. In-whisker growth was accompanied by an increase in oxygen content in the films. The morphology and extrusion kinetics of In-whiskers were affected by the local chemical composition. The results presented here enable controlled processing of one-dimensional nanostructured materials with respect to morphology and growth kinetics.

Zusammenfassung

Ab initio-Berechnungen von Perovskiten der allgemeinen Formel AB_3X, wobei *A* und *B* Metalle sind und *X* für eines der Elemente B, C oder N steht, lassen auf außergewöhnliche mechanische Eigenschaften dieser Stoffklasse schließen, insbesondere eine hohe Duktilität und somit hohe Schadenstoleranz.

Im ersten Teil dieser Arbeit wird das mechanische Verhalten ternärer, perovskitischer Boride und Nitride untersucht. YPd_3B-, Fe_4N-, $ZnFe_3N$- und $PdFe_3N$-Schichten wurden mittels kombinatorischem Magnetronsputtern synthetisiert und ihre mechanischen Eigenschaften mittels Nanoindentation bestimmt. Der Vergleich der gemessenen Werte für den Elastizitätsmodul zeigt eine gute Übereinstimmung mit den ab initio-Daten. Aus der Analyse der kritischen Scherspannung zur Aktivierung plastischer Verformung wird geschlossen, dass YPd_3B, Fe_4N und $PdFe_3N$ als duktile Werkstoffe einzustufen sind. Dies ist ebenfalls konsistent mit den Ergebnissen der ab initio-Berechnungen.

Der zweite Teil der Arbeit befasst sich mit der Evaluierung der potentiellen Anwendung der kombinatorischen Dünnschichtsynthese zur Herstellung eindimensionaler nanostrukturierter Werkstoffe. In-Y-Dünnschichten wurden über einen großen Zusammensetzungsbereich mittels kombinatorischem Magnetronsputtern abgeschieden. Bei anschließender Auslagerung der Dünnschichten an Luft wurde die spontane Extrusion von In-Whiskern aus der der Schicht beobachtet. Das Whisker-Wachstum korreliert mit einem Anstieg des Sauerstoffgehalts der Schichten. Die Morphologie und die Wachstumskinetik der Whisker werden direkt durch die lokale chemische Zusammensetzung beeinflusst. Die hier erarbeiteten Zusammenhänge zwischen dem Bildungsmechanismus, der

Wachstumskinetik und der Whiskermorphologie leisten einen Beitrag zur gezielten Herstellung eindimensional nanostrukturierter Werkstoffe.

List of publications contributing to this thesis work

T. Takahashi, A. Abdulkadhim, D. Music, and J.M. Schneider
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