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New quaternary amorphous materials
Si-B-C-N: reactive magnetron sputtering and
an ab-initio study

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To the best of my knowledge, this thesis contains no copy or paraphrase of work published by any other person, except where duly acknowledged in the text.

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New quaternary amorphous materials Si-B-C-N: reactive magnetron sputtering and an ab-initio study

First part of the thesis is focused on experimental preparation of new hard quaternary amorphous materials Si-B-C-N with high thermal stability. Materials were prepared in the form of thin films using reactive magnetron sputtering. The technique used proved to be suitable for reproducible synthesis of these materials. The Si-B-C-N films were generally found to be amorphous with low compressive stress and good adhesion to silicon or glass substrates. The process and film characteristics were controlled by varying the sputter target composition, the Ar fraction in the N₂-Ar gas mixture, the negative rf-induced substrate bias, and the substrate temperature. Main conclusions describe the relationships between process parameters, discharge and deposition characteristics and film properties (elemental composition, chemical bonding structure, material hardness, compressive stress or electrical conductivity of materials prepared).

Second part of the thesis is focused on ab-initio simulations of structures of experimentally prepared Si-B-C-N materials. In the performed liquid-quench simulations, the Kohn-Sham equations for the valence electrons are expanded in a basis of plane wave functions, while core electrons were represented using Goedecker-type pseudopotentials. We simplified the ion bombardment process by assuming that the primary impact creates a localized molten region of high temperature and sufficiently short cooling time, commonly referred to as a thermal spike. Main conclusions deal with N₂ formation in studied materials, effect of implanted Ar on structure and properties of prepared materials, ability of Si to relieve that part of compressive stress which is caused by implanted Ar, and ability of B to improve thermal stability of Si-B-C-N materials. The calculated results are compared with experiment.

Nové kvaternární amorfni materiály Si-B-C-N: reaktivní magnetronové naprašování a ab-initio studie

První část disertace se zabývá experimentálním vytvářením nových tvrdých kvaternárních amorfni materiálů Si-B-C-N s vysokou teplotní stabilitou. Materiály byly připravovány ve formě tenkých vrstev pomocí reaktivního magnetronového naprašování. Použitá metoda se ukázala jako velmi vhodná pro reprodukovatelnou přípravu těchto materiálů. Vytvořené materiály Si-B-C-N byly obecně amorfni s nízkým kompresním pnutím a dobrou adhezí ke křemíkovým i skleněným substrátům. Depoziční proces a vlastnosti vytvořených materiálů byly řízeny složením rozprašovaného terče, složením výbojové směsi N₂-Ar, negativním rf předpětím na substrátech a teplotou substrátů. Hlavní závěry popisují vztahy mezi procesními parametry, charakteristikami depozičního procesu a vlastnostmi vytvořených materiálů (prvkové složení, vazebná struktura, kompresní pnutí a elektrická vodivost).

Druhá část disertace se zabývá ab-initio výpočty struktur experimentálně připravených materiálů Si-B-C-N, pomocí tzv. liquid-quench simulačního algoritmu. Kohn-Shamovy rovnice pro valenční elektrony byly řešeny s využitím rozložení vlnové funkce valenčních elektronů na rovinné vlny, zatímco jádra atomů a vnitřní elektronové orbitály byly popsány pomocí Goedeckerových pseudopotenciálů. Iontový bombard byl zjednodušeně popsán na základě předpokladu, že dopad iontu vede k lokálnímu roztavení a následnému dostatečně rychlému zchlazení malého objemu materiálu – tzv. thermal spike. Hlavní závěry popisují vytváření molekul N₂ ve studovaných materiálech, vliv implantovaných atomů Ar na jejich strukturu a vlastnosti, schopnost Si snížit kompresní pnutí indukované atomy Ar, a schopnost B zvýšit teplotní stabilitu materiálů Si-B-C-N. Vypočítané výsledky jsou porovnávány s experimentálními.

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