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Vacancies and Thermodynamics in Al-O-N and Al-Si-N Thin Films

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Ternary Aluminum Oxynitride (Al-O-N) and Aluminum Silicon Nitride (Al-Si-N) as well as the quaternary combination Aluminum Silicon Oxynitride (Al-Si-O-N) can be fabricated as thin coatings by Reactive Unbalanced Closed Field Direct Current Magnetron Sputtering (R-UCFDCMS). They all provide attractive qualities such as full transparency and hardness, which renders them interesting as e.g. transparent protection layers.

Low amounts of O and Si can be considered as dopant atoms that incorporate the AlN wurtzite lattice. O replaces N on anionic lattice sites, since both of these atoms are electronegative and thus act as electron acceptors. Si, on the other hand, exchanges with electron donating Al. The result is a crystalline solid solution. The substitutions lead to an electron excess, because both dopants contain one valence electron more than the atoms they replace. A potential mechanism to account for this electronic imbalance is the formation of Al vacancies on cationic lattice sites. As a supporting indication for voids, cell lattice parameters measured by X-ray diffraction are observed to shrink upon O and/or Si addition. To consolidate the hypothesis, ab initio DFT calculations were performed. Cell parameter changes upon solid solution formation were calculated and showed good agreement with experimental results. The solid solution was also tested for its thermodynamic state and found to be metastable.

Upon raising the O and/or Si content and transgressing the solubility limit found at 6-8% O and/or Si, a nanocomposite forms. The single crystallites are continuously enveloped in an amorphous tissue of Al₂O₃ and/or Si₃N₄. At yet higher O and/or Si portions above 30%, the material develops into a fully amorphous phase.

Keywords

aluminum silicon oxynitride
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solid solution
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