Epitaxy of Single Crystal Thin Film Earth-Abundant Element Heterovalent Nitride Semiconductors for Tandem Cell.

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Interest in earth-abundant element compound semiconductors has yielded a sizeable number of candidate materials suitable for optoelectronic devices, including those intended for photovoltaic applications. One interesting family of potential materials is analogous to III-V semiconductors in the same way that CIGS is analogous to the II-VI compounds, in that pairs of column III metallic elements are replaced by a pair of column II and column IV elements. In particular, the nitride members of this class of materials has attracted attention recently, with ZnSnN2 showing promise as an alternative to indium-rich InGaN.

We have demonstrated high-quality single crystal thin films of ZnSnN2 using plasma-assisted molecular beam epitaxy (MBE), and measured structural, optical and electronic properties. Somewhat unexpectedly, we observed that it is possible to alter the periodicity of the cation sublattice, and in so doing, can switch between the orthorhombic and wurtzite lattice structures by varying the growth parameters [1]. Intriguingly, in a fashion similar to what has been observed in other cation disordered compounds, the band gap of the material changes significantly between the two lattice structures, with a predicted range of approximately 1 to 2 eV. Experimentally, we have already observed optical band gaps in the range of 1.3 to 2.3 eV, although both values are affected by the Burstein-Moss effect as the very thin (~150 nm) samples are degenerately n-type. While the majority of films have been grown on (111) YSZ, we will also report the results of experiments using LiGaO2, which has a closer lattice match to the orthorhombic structure and appears to stabilize that symmetry more easily. It is worth noting that in addition to MBE, a number of groups have successfully deposited high-quality thin films using other techniques [2], including sputtering.

Beyond ZnSnN2, which is of interest for terrestrial photovoltaics depending on the crystal structure and corresponding electronic band gap, there are also several closely related materials which could be of interest for short wavelength applications. Among these is ZnGeN2, which has been estimated to have a band gap of approximately 3.3 eV (very close to that of GaN). We have recently conducted preliminary growth experiments on this material using several substrates including YSZ, and noted that growth behavior appears to mirror that of $ZnSnN_2$.

References:

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