Critical thickness and misfit dislocations in rocksalt ZnMgO layers grown on MgO (100)

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Zinc oxide has wurtzite structure (wz-ZnO) at ambient conditions. Due to the promising bandgap (4.0-7.8eV) we consider the misfit stress for the growth of rock salt $Zn_xMg_{1-x}O$ layers on rock salt MgO. At ambient conditions, a solid solution of ZnO in MgO is stable only up to 13%. Nevertheless, due to the misfit stress the range of chemical composition of thermodynamically stable layers can be extended.

We consider a mechanism of dislocation network formation at the interface rs-$Zn_xMg_{1-x}O$/MgO. Based on the dislocation theory, many different analytic formulas for critical layer thickness have been derived, cf. Hu (1991), Brown (2002). The formulas concern the critical thickness of the layers which retain thermodynamically stable at atmospheric pressure. On the other hand, for thin layers which lose the stability earlier, before the stress relaxation, we can expect a lower critical thickness. We present a derivation of an analytic formula for the critical thickness of rs-$Zn_xMg_{1-x}O$ layers which lose the stability due to the rocksalt-wurtzite phase transition, cf. Lu et al. (2016). In the new formula the dependency of the onset elastic energy $E(\sigma,x)$ of the rs-wz phase transition is taken into account. In the general case this energy depends on the misfit stress and chemical composition.

Hu, S.M. (1991) J. Appl. Phys. 69, 7901–7903.
Braun, A., at al. (2002) J. Cryst. Growth, 241, 231–234.
Lu, C.-Y.J. et al. (2016) J. Chem. Phys. 144, 214704.