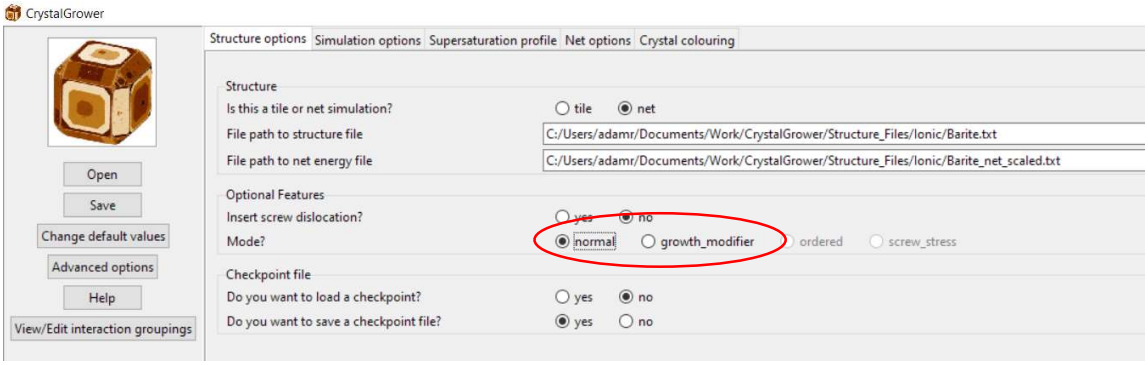
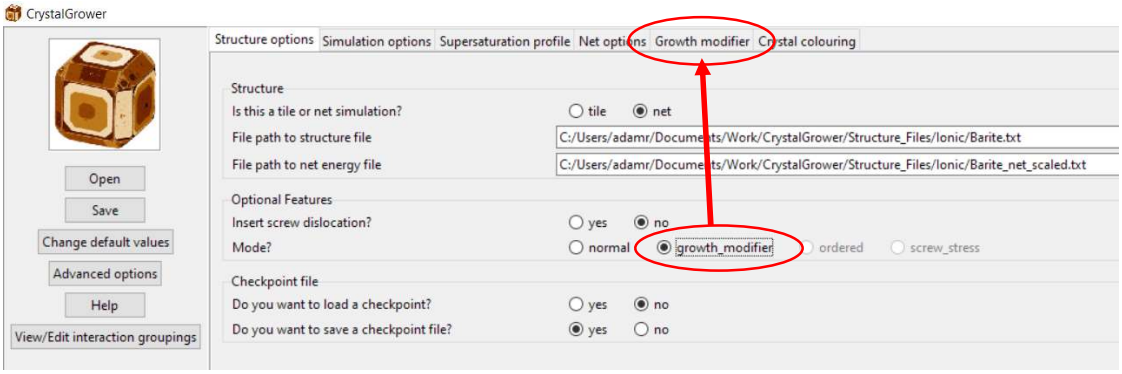
Setting the Simulation Behaviour Mode

Mode?: this refers to the type of simulation required. By default this is set to normal. If you want to add growth modifiers to poison sites check "growth modifier". In that case a new tab [Growth Modifier] will appear where information about the sites to be poisoned is entered. Additional modes currently being tested are "ordered" - for consideration of the order of framework atoms in "tile" structures and "screw_stress" - to model the addition of stress at the screw core. Please enquire on the Contact Us page to arrange a possible collaboration using these modes.

The modes offered here are designed to replicate general behaviours seen across a number of simulation types. “normal” is used to simulate standard crystallisation behaviour, generally in solutions without impurities.



“growth_modifier” simulations are to be used in situations where molecular impostors / poisoning agents / growth modifiers are added to a solution of crystallising material. An additional tab is created for controlling the behaviour of the growth modifier. Please consult the detailed growth modifier section of the manual for more information.



Two additional modes are currently in development to be added to *CrystalGrower* in the near future.

The “ordered” mode is designed for framework solids where it is necessary to consider the order of framework atom incorporation into the solid.

The “screw_stress” mode is designed to model screw dislocations where strain is exhibited near the screw dislocation core as the free energy of the solid phase is raised relative to the solution phase. This functions like a targeted poison at a set distance around the screw core.

If users are interested in using the new modes to model specific features observed in their crystals, collaborations can be arranged by contacting our research group at the University of Manchester.