* at concentration X:
  + create initial solid alloy structure
  + run nve, and npt and desired starting temp and pressure, save the final structure, A
  + melt A: while allowing z dimension to vary, increase temp to 3000K, and anneal down to desired starting temp, save the final structure, B
  + concatenate A and B, with box enclose everything + crystal constant
  + MI
    - run nve, and npt at temp a
    - run nve, and npt at temp b
    - run nve, and npt at temp c
    - run nve, and npt at temp d
    - run nve, and npt at temp e
    - run nve, and npt at temp f
    - run nve, and npt at temp g