Monte Carlo simulations of self-organising nanostructures in PbTe/CdTe multilayer system

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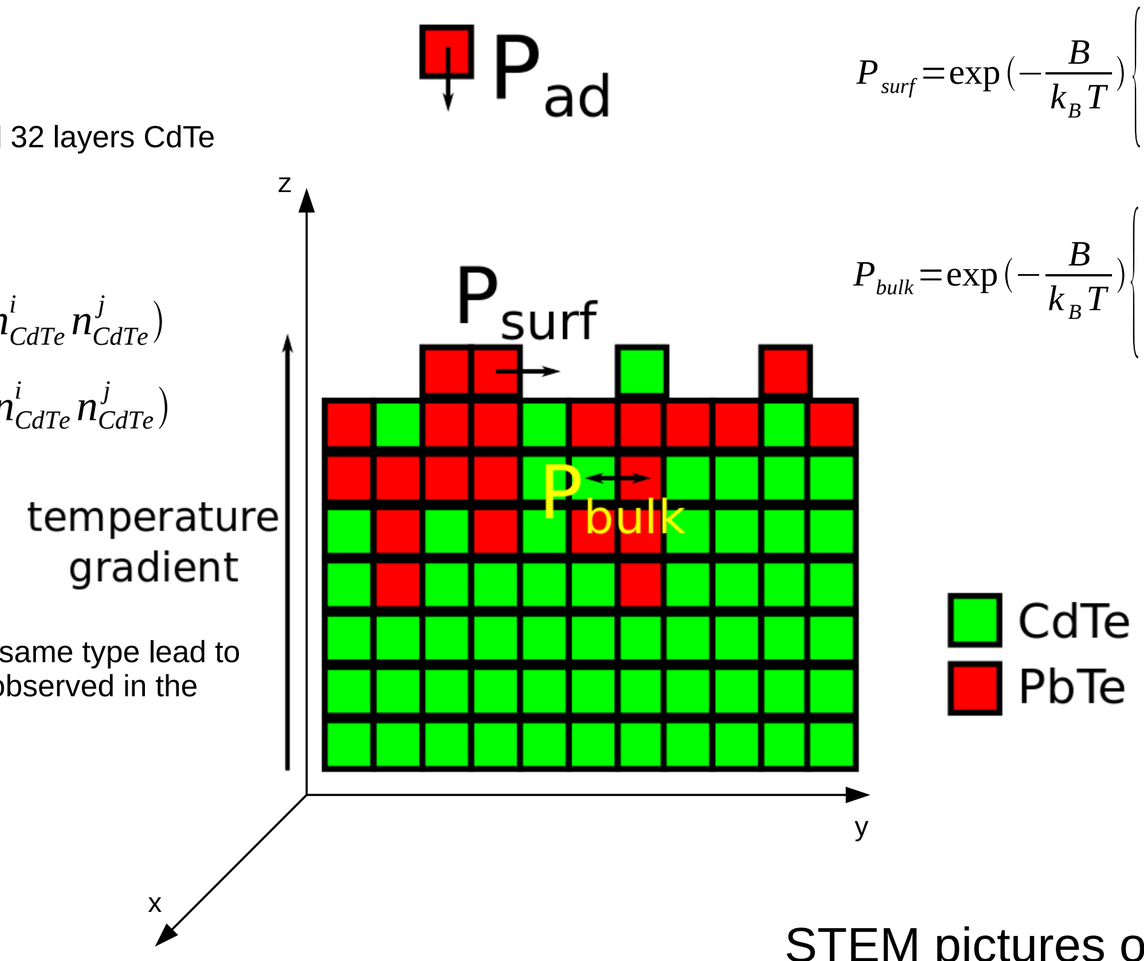
We propose a simple lattice gas model of crystal growth involving two different components. This study is motivated by various experiments concerning immiscible systems, that is systems of two components that do no mix with each other but instead create various structures such as quantum dots or nanowires of one of the materials embedded in the other one. Examples of such systems are PbTe/CdTe structures[1-4]. We perform Monte Carlo simulations based on our model and compare their results with those obtained in the experiment of PbTe/CdTe multilayer growth in different temperatures[2].

3D lattice gas model of two-component crystal growth

Alternate growth of 12 layers PbTe and 32 layers CdTe for several repetitions

$$H = -J_{nn} \sum_{\langle i;j \rangle}^{nn} \left(n^i_{PbTe} n^j_{PbTe} + n^i_{CdTe} n^j_{CdTe} \right) - J_{nnn} \sum_{\langle i;j \rangle}^{nnn} \left(n^i_{PbTe} n^j_{PbTe} + n^i_{CdTe} n^j_{CdTe} \right)$$

Attractive forces between the particles of the same type lead to immiscibility of the components, which is observed in the experiments.



$$P_{surf} = \exp\left(-\frac{B}{k_B T}\right) \begin{cases} \exp\left(-\frac{\Delta E}{k_B T}\right) & \Delta E \geq 0 \\ 1 & \Delta E < 0 \end{cases}$$

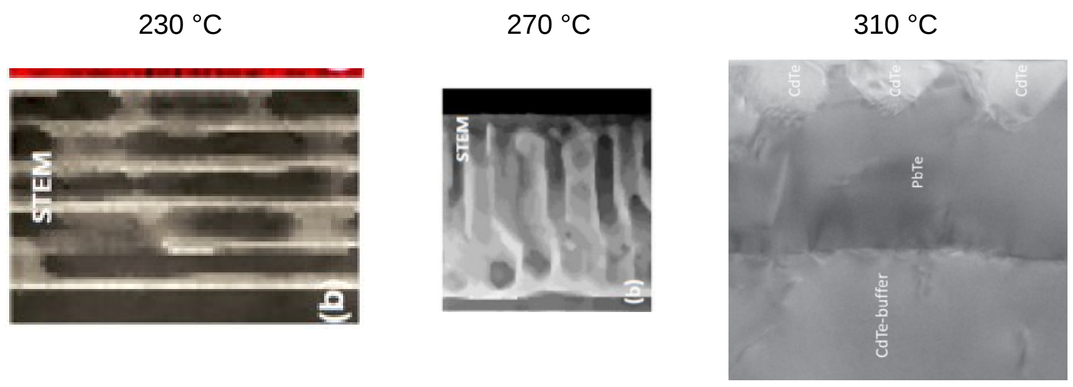
$$P_{bulk} = \exp\left(-\frac{B}{k_B T}\right) \begin{cases} \exp\left(-\frac{\Delta E - k(z_1 - z_0)}{k_B T}\right) & \Delta E - k(z_1 - z_0) \geq 0 \\ 1 & \Delta E - k(z_1 - z_0) < 0 \end{cases}$$

ΔE – energy change due to the jump
T – temperature of the system
k – bias towards the growth direction (temperature gradient)
B – energetic barrier for a single jump

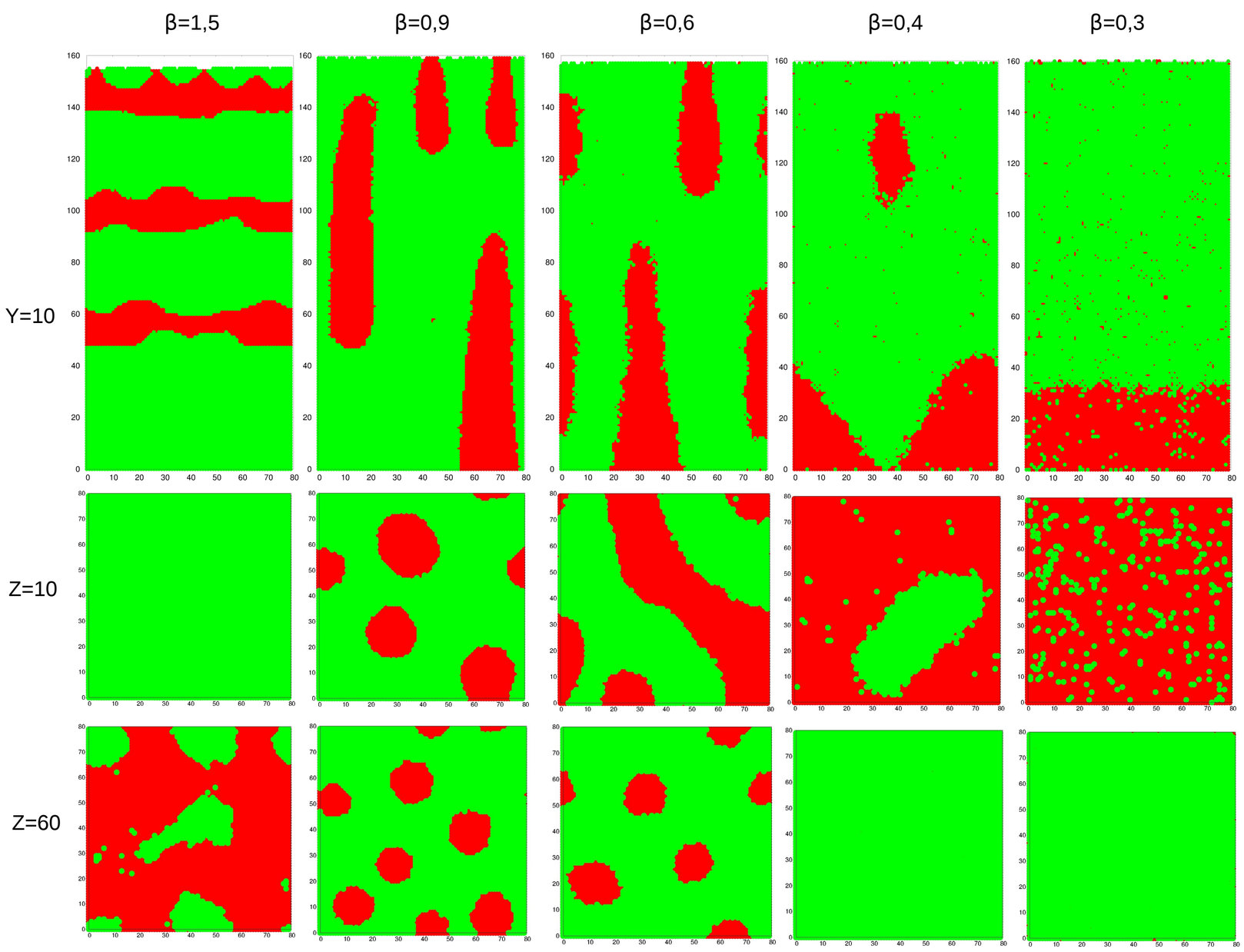
Monte Carlo simulations of PbTe/CdTe structures

One Monte Carlo step:
- PbTe or CdTe particles are adsorbed with probability P_{ad}
- Bulk diffusion is realised by changing the positions of two randomly chosen neighbouring particles of different type
- Surface diffusion is realised by moving a randomly chosen particle on the surface

STEM pictures of PbTe/CdTe structures grown in the experiment[2]



J_{nn}=0,22 J_{nnn}=0,66 k_{PbTe}=0,5 k_{CdTe}=0,55



Conclusions

·We have simulated multilayer PbTe/CdTe growth in different temperatures.
·At low temperatures the obtained structures were as expected, that is 2D horizontal layers.
·At middle temperatures columns of PbTe embedded in CdTe were formed and their diameter increased with temperature.
·At high temperatures complete separation of both materials was observed.
·The observed structures are in agreement with the experiment[2].

References

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