Matching Rules
from Al-Co Potentials
in an almost realistic model

Sejoon Lim, Marek Mihalkovič, and Christopher L. Henley,
[Support: U.S. DOE and (M.M.)
VEGA 2/0157/08 and APVV-0413-06]

Zurich, July 8 2008
Outline

1. Basics

   The model; simulation results

2. Evolution of order/ diagnostics

   Potentials $V_{AB}(R)$; 4 aspects/stages of ordering

   2 diagnostics (1) $\Delta E(R)_{T,T'}$ (2) change $R_{\text{cutoff}}$

3. Whence Penrose rules? (A. From $V_{\text{AlCo}}(R)$ at 2nd neighbor)

   Energy cost: via 4 Å Co-Co supertiling

4. Discussion

   Relaxation/ab-initio; breakdown in Al-Ni case (also Al-Cu-Co)
1.1 Our simulation recipe

[Mihalkovic - Widom - Henley et al, 2002, 2006:] $d$(AlNiCo).

Inputs:

(1) realistic pair potential

(2) assume layering ($c/2 = 2.04 \text{ Å};$ period $c$)

(3) assume discrete sites ($a_r = 2.455\text{Å}$)

Discover structure by stages:

(a) unconstrained MC w/lattice gas

(b) infer deterministic decoration of larger tiles

\[\rightarrow\] do “constrained” tile MC w/ Hamiltonian

This project: Al$_{80}$Co$_{20}$ binary
1.2 Simulation results

a). Unconstrained (lattice-gas) simulation

(Nearly) perfect Penrose HBS tiling.

Except:
“pseudo-vacancy”
(Al corner with no Co neighbors becomes vacant)

Two kinds of violations are shown.
V-rule (marked by V) and Fat/Fat (marked by O).
HBS tiles and Penrose arrows

Satisfy (only) double arrows:
HBS = composites of rhombi

HBS tiles are realized in most Al-TM decagonals:
⇒ need worry only how single-arrow edges satisfied
1.3 Constrained (tiles) simulation
(w/o pseudovacancy)

Penrose tiling! (except 4 defects/cell forced by periodic b.c.)
2.1 Al-TM potentials: key features?

- a) $V_{\text{Al-Al}}(R)$: mainly n.n. repulsion; weak at long range
- b) $V_{\text{Al-TM}}(R)$: strong attraction near 2.45 Å.

We will relate these to four aspects of ordering.

Al-Al and Al-TM (2.5–3):
HBS tiling
TM-TM (~4.5): TM supertiling
Al-TM (3.8-4.7): matching rules
2.2 Evolution of order: higher T

Aspect (2) TM-TM (nearly HBS) supertiling ($\tau a_r \approx 4.0\text{Å}$)

Due to 2nd neighbor TM-TM.

CLICK 2nd version with overlay of Co-Co HBS

MOVE The relative no. of Boat versus Star tiles depends on the Al content. (Important: it must be the Penrose ratio $\sqrt{5} : 1$.)
2.3 Diagnostics?
3.1 Whence matching rules?

Aspect (3) Fat/Thin matching: “V-rulea”

2nd nbr Al-TM ⇒ correct arrows

Example
(note Fat Hexagon around “V”)

Result is **V-rule**: pair every Fat-Fat concave corner ↔ every Thin convex corner.
(Possible, iff Penrose number ratio Boat/Star.)

Note no. of 2nd-nbr TM-TM interactions is same in all HBS tilings satisfying the V-rule so **don’t** affect matching rules
Aspect (4) Fat/Fat rhombus matching rule:

Fat rhombus with edges left over from V-rule always contain an internal Al atom. Satisfying the arrows gives one more (favorable) 4.46Å Al-Co bond.

2nd nbr Al-TM ⇒
correct Fat-Fat arrows

Note no. of 2nd-nbr TM-TM interactions is same in all HBS tilings satisfying the V-rule, so don’t affect matching rules.
4.1 Discussion: other systems?
4.2 Summary

Rather realistic interactions and a (nearly) realistic composition organized into a Penrose tiling with matching rules.

Due mainly to Al-TM attractive well at $R \approx 4.5\,\text{Å}$. Many interactions contribute to rules, but mostly of same sign (not “frustrated”)

Penrose case has shortest interaction radius $R_{\text{min}}$ needed to distinguish valid from defective tilings

Crucial to tune the Al content (fortunately it’s robust)
4.3 Future directions?

Mathematical proofs?

Real Al-TM systems:

Other tiles (e.g. Decagon in Co-rich Al-Co-Ni) disrupt m-rules.

“Puckering”: interior Al in HBS tiles deviate off planes; stacking period doubles ($\rightarrow 2c$).

Role in real decagonals:
may encourage supertiles which are built from small tiles as in Penrose, even if the final answer is not a Penrose tiling.