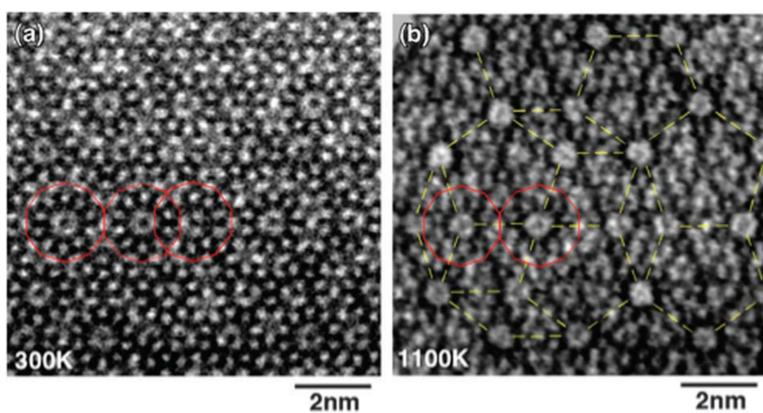


Introduction

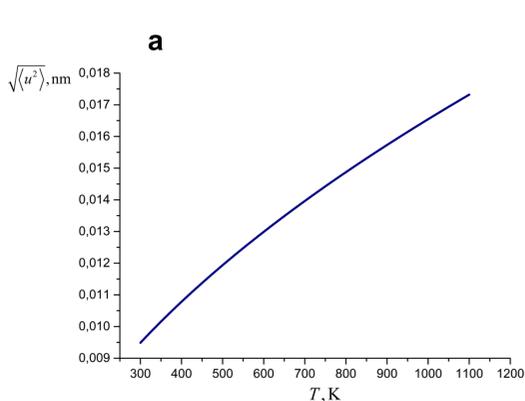
Among many surprising properties of quasicrystals (QC) is their high catalytic activity. An important parameter of the chemical kinetics is the *activation energy*, i.e. the energy required to overcome the reaction barrier. The lower is the activation energy, the faster the reaction rate, and so a catalyst may be thought to reduce somehow the activation energy. Recently, it has been shown that in a crystalline matrix, the activation energy may be reduced at some sites due to a special class of *localised anharmonic vibrations* (LAVs) of atoms, known also as *discrete breathers* or *intrinsic localized modes*. LAVs can be excited either thermally or by external driving, resulting in a drastic acceleration of the reaction rates in their vicinity.

In this context, we present atomistic simulations of LAVs in 1-D QCs and a model of catalysis in QC that can take place at special sites provided by their inherent topology. A striking *site selectiveness* of LAV formation in disordered structures and small clusters allows one to suggest that their concentration in quasicrystals may be very high as compared to regular crystals where LAVs arise homogeneously. Direct experimental observations of LAVs in the decagonal quasicrystal $\text{Al}_{72}\text{Ni}_{20}\text{Co}_8$, have shown that they are arranged in just a few nm from each other. So in this case, one deals with a kind of 'organized disorder' that stimulates formation of LAVs, which may explain a strong catalytic activity of some quasicrystals.

Site selectiveness of LAV formation in $\text{Al}_{72}\text{Ni}_{20}\text{Co}_8$.

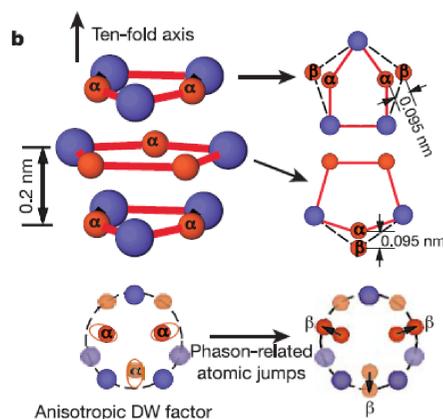


STEM images of **LAVs** of the decagonal $\text{Al}_{72}\text{Ni}_{20}\text{Co}_8$ at (a) 300 K and (b) 1100 K, according to **Abe et al (2003)**. Connecting the center of the 2 nm decagonal clusters (red) reveals significant temperature-dependent contrast changes, a pentagonal quasiperiodic lattice (yellow) with an edge length of 2 nm can be seen in (b)



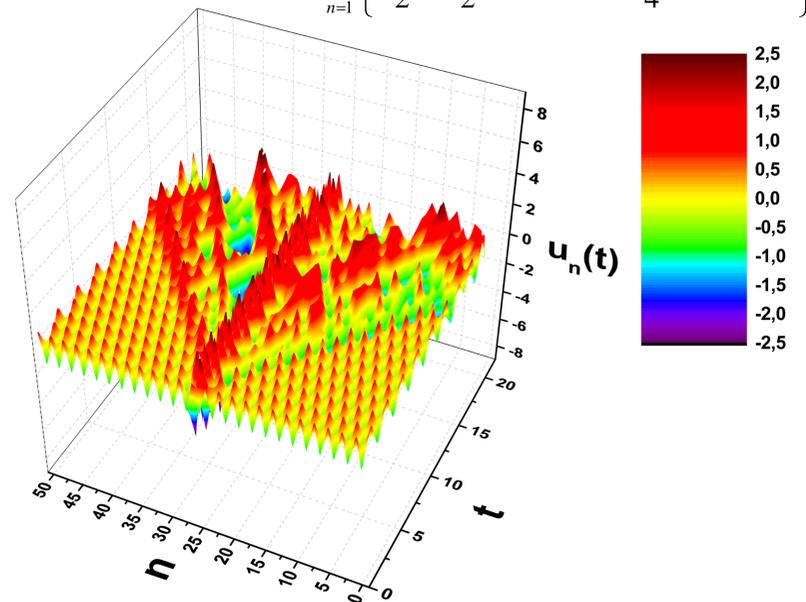
(a) **LAV** amplitude dependence on temperature in $\text{Al}_{72}\text{Ni}_{20}\text{Co}_8$, fitted by two points at 300 K and 1100 K, according to **Abe et al (2003)**. The maximum LAV amplitude $A_{\text{LAV}}(1100\text{K}) = 0.018$ nm.

(b) **LAVs** give rise to **phasons** at $T > 990$ K, where a phase transition occurs, and additional quasi-stable sites β arise near the sites α . The phason amplitude $A_{\text{ph}}(1100\text{K}) = 0.095$ nm is an order of magnitude larger than that of LAVs.



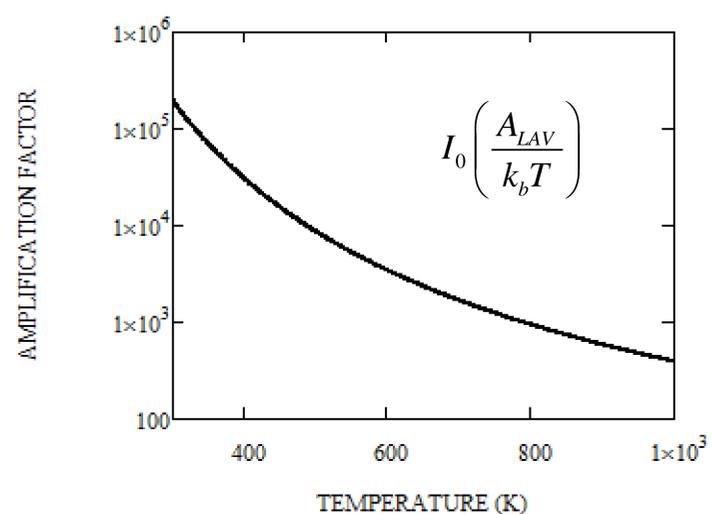
Atomistic simulations of LAVs in 1-D QCs

Hamiltonian of the system:
$$H = \sum_{n=1}^N \left\{ \frac{m\dot{u}_n^2}{2} - \frac{1}{2}(u_n - u_{n-1})^2 + \frac{1}{4}(u_n - u_{n-1})^4 \right\}$$



The displacement of the n -th atom as a function of the site number n and time t . **LAV** is localized on the 25-th and 26-th sites.

LAV-induced amplification of reaction rates in QC



Temperature dependence of the Amplification Factor according to [2] with **LAV** amplitude A_{LAV} deduced from [1]

- [1] E. Abe, S.J. Pennycook, A.P. Tsai, *Direct observation of a local thermal vibration anomaly in a quasicrystal*, Nature (London), 421, (2003) 347.
 [2] V. I. Dubinko, P. A. Selyshchev, J. F. R. Archilla, *Reaction-rate theory with account of the crystal anharmonicity*, Phys. Rev. E 83 (2011) No 4

Conclusions/outlook

- The present model explains high catalytic activity of **QC** by linking it to **LAV-induced** catalytic mechanism.
- LAV formation has been demonstrated in 1-D **QC** by means of numerical modelling and in 3-D decagonal $\text{Al}_{72}\text{Ni}_{20}\text{Co}_8$ by means of ultrahigh resolution transmission electron microscopy (STEM)
- Atomistic modeling of LAVs of various types in **QC** is an important outstanding problem since it may offer new ways of *engineering catalysts*.