# Role of defective icosahedra in undercooled metals

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Undercoolings as large as 20% of the melting temperature is observed for a great variety of different metals.

Even in simple liquids the short range order may differ from that of crystalline solids.

Icosahedral short range order is postulated in the melts to explain the large undercoolings of pure metals.

Recent experimental literature:

- Di Cicco *et al.*, PRL 2003
- Kelton *et al.*, PRL 2003
- Schenk *et al.*, PRL 2002

A commons approach is to characterize the liquid metal by starting from the analysis of the single icosahedra and its deformations.

## Icosahedra

13 atoms 55 atoms 147 atoms

Computing the energy by using Lennard-Jones interatomic potential, 13 atom icosahedra energy is about 8% smaller than corresponding fcc and hcp structure.

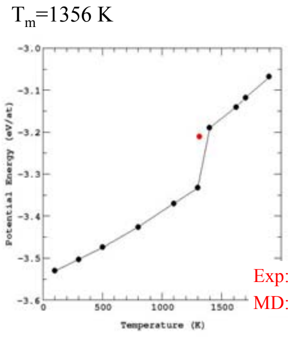
## Computational details

Classical Molecular Dynamics simulations of 4000 copper atoms. Constant temperature and constant pressure simulations

$$E_c = \sum_i E_R^i + E_B^i \qquad \begin{cases} E_B^i = -\left\{ \sum_j \xi^2 e^{-2q(r_{ij}/r_o - 1)} \right\}^{1/2} \\ E_R^i = \sum_j A e^{-p(r_{ij}/r_o - 1)} \end{cases}$$

Cleri and Rosato, PRB 93

$T_m$=1356 K



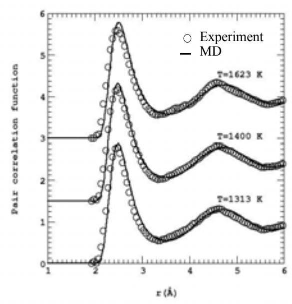

Temperature of interest:
Liquid: T= 1623 K and T=1400 K
Undercooled: T=1313 K

T=1623 K : L=38.47 Å
T=1400 K : L=38.14 Å
T=1313 K : L=30.01 Å

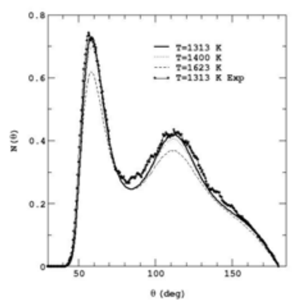
<5% of difference with experimental densities

Exp: D=3.97 10-5 cm2/sec at $T_m$=1356 K
MD: D=3.90 $10^{-5}$ $cm^2$/sec at T=1400 K

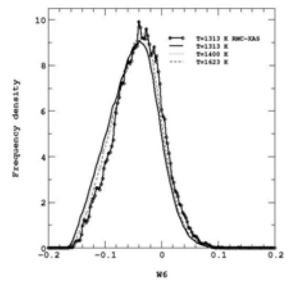
## Pair correlation



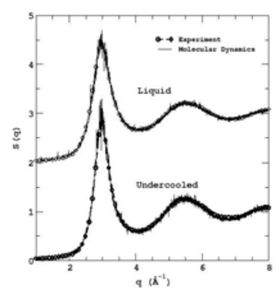

## Bond angle distribution




## $W_6$ analysis




## Neutron structure factor




Liquid:
Exp: T=1833 K
MD: T=1623 K
Undercooled:
Exp: T=1393 K
MD: T=1313 K

O.J. Eder *et al.*, J. Phys. F: Metal. Phys. 1980

## Common neighbor analysis

Three indeces *jkl* specifies the local environment of a pair of atoms:

*j* = the number of neighbors common to both atoms
*k* = the number of bonds between the common neighbors
*l* = the number of bonds in the longest continuous chain formed by the k bonds between common neighbors

Ref: Clarke and Jonsonn (PRE 93)

For example:

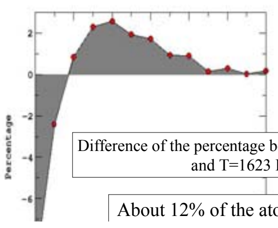
**555** → icosahedral order
**421** → fcc order
**421** and **422** → hcp order

ICOSAHEDRAL cluster has the central atom characterized by 12 nearest neighbor atoms with 555 environment

$N_{555}$ = 12

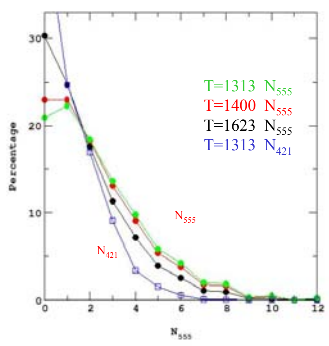
**PERCENTAGES**

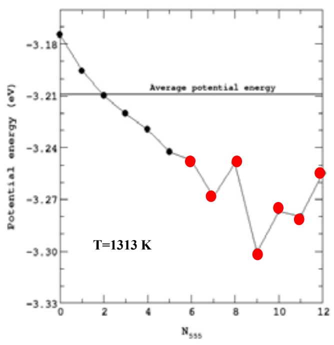
| $N_{555}$ | T=1623K | T=1400K | T=1313K |
|---|---|---|---|
| 0 | 30.32 | 22.99 | 20.90 |
| 1 | 24.67 | 22.99 | 22.27 |
| 2 | 17.57 | 18.29 | 18.40 |
| 3 | 11.33 | 13.12 | 13.63 |
| 4 | 7.19 | 9.07 | 9.77 |
| 5 | 3.92 | 5.40 | 5.85 |
| 6 | 2.53 | 3.81 | **4.26** |
| 7 | 1.10 | 1.81 | **2.03** |
| 8 | 0.93 | 1.61 | **1.86** |
| 9 | 0.14 | 0.26 | **0.29** |
| 10 | 0.20 | 0.41 | **0.48** |
| 11 | <0.01 | <0.01 | **<0.01** |
| 12 | 0.11 | 0.22 | **0.26** |




Difference of the percentage between T=1313 K and T=1623 K

About 12% of the atoms change



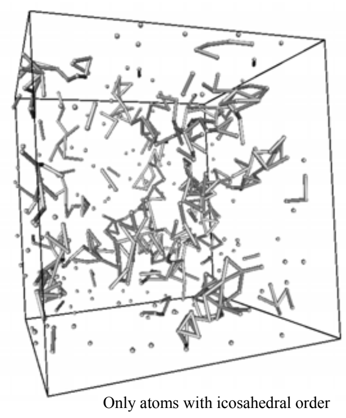

## CONCLUSIONS

Icosahedral short range order is present in liquid and undercooled metals

The number of icosahedral atoms increases cooling the systems.

Not regular clusters are formed in the undercooled by icosahedral atoms.

More than 70% of the atoms are involved in in icosahedral short range order.



Only atoms with icosahedral order