ON IMPORTANCE OF THE MULTI-LEVEL CHEMICAL OBJECTS DESCRIPTION IN ONTOLOGIES FOR INFORMATION SYSTEMS INTEGRATION IN INORGANIC MATERIALS SCIENCE

Dudarev V.A.,* Kiselyova N.N.

IMET RAS, Moscow, Russia

**vic_dudarev@mail.ru*

In past years ontologies (on OWL) usage becomes popular for problem domains description and creating basis for thematic information systems (IS) integration. For example, in inorganic materials science several ontologies are known to consolidate information [1] [2]. One of their significant drawbacks is an unjustified description simplification for substance (or material).

The importance of multilevel chemical object description is shown by the example of IS developed in IMET RAS. ¡¡Diagram¿¿ IS (`http://diag.imet-db.ru`) describes phase diagrams of double and triple chemical systems. In another ¡¡Crystal¿¿ IS properties are described at other detail levels of chemical objects: the melting temperature is described at the substance (or compound) level, and the hardness — at its crystal structure information level [3].

Thus, developing the ontology for IS information integration on inorganic substances properties, it is necessary to implement means for properties definition at different levels of chemical objects description and to ensure an automatic matching for the upper-level hierarchy properties with the current chemical object.

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