Non equilibrium transformations of molecular compounds induced mechanically

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Contrary to metallurgy, systematic investigations of the mechanically induced transformations of molecular compounds have not yet been done. However there is a strong interest to get a better understanding of these transformations for both practical (in pharmacy, agrochemistry, dyes…) and fundamental reasons.

There are several specific properties of molecular compounds which have special relevance in mechanical activation. Their molecular and crystalline symmetry are generally low, they are good glass former, their melting and glass transition temperatures are low, the inter molecular interactions are week… All these specificities lead to expect a strong sensitivity of molecular compounds to the intensity and temperature of grinding. From a fundamental point of view molecular compounds certainly offer new interesting situations which allow testing theoretical approaches.

In this communication we present some selected results which may help clarifying the behaviour pattern of molecular compounds under grinding.

The whole set of experiments can be interpreted in the framework of the driven material concept. According to this model the process involves a competition between ballistic disordering process which is independent of temperature and a thermally activated restoration. The transformations which are induced by grinding are thus nonequilibrium transformations towards dynamic stationary states rather than towards thermodynamic equilibrium states. This allows proposing some possibilities to control the transformations. Either grinding can amorphize (Fig. 2) a compound or convert it to an other polymorphic crystalline phase (Fig. 1).

Two other aspects of opportunities provided by grinding molecular compounds will be considered namely:

(1) The possibility to manipulate the degree of aging of the amorphous state itself.

(2) New possibilities to create glass solutions.

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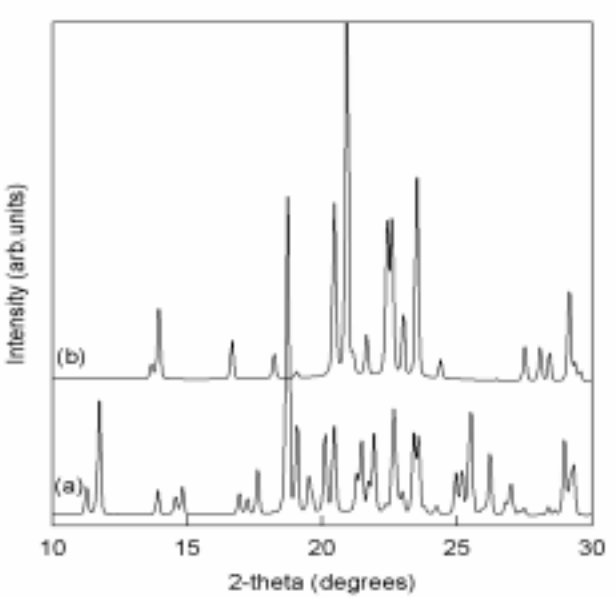

Fig. 1 X-ray diffraction patterns of sorbitol recorded at room temperature before milling (a) and after 10 hours of milling treatment (b)

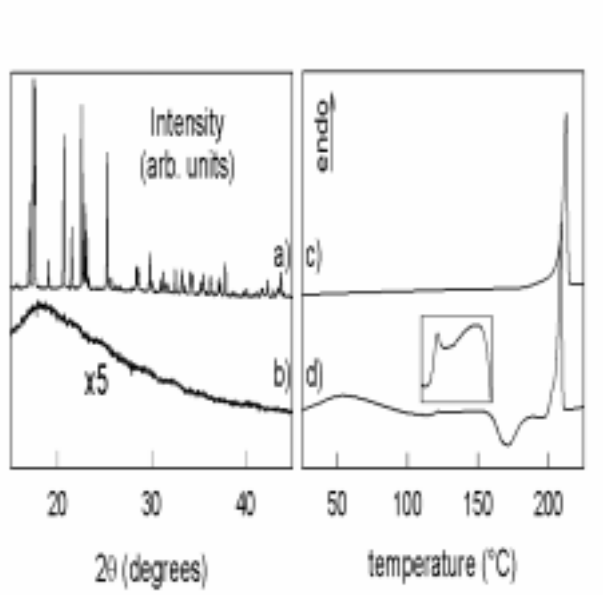

Fig. 2 X-ray diffraction patterns of trehalose recorded at room temperature before milling (a) and after 20 hours of milling treatment (b). DSC heating curves (5°C/min) of crystalline trehalose before milling (c) and after 20 hours of milling treatment (d).The curve in inset is a close up view of the glass transition domain of curve d.

References

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