



South Bohemian
Research Center
of Aquaculture
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Name of software (Czech): Cubic-elestic

Name of software (English): Cubic-elestic

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Description (Czech):

Softwarový balíček pro výpočet elastických tensorů z kubické struktury pomocí derivací druhého řádu v kódu Wien2k, tento balíček počítá přesné hodnoty elastických konstant v kubickém systému. Výsledky získané pomocí tohoto balíčku jsou ve velmi dobré shodě s měřením. Další podrobnosti jsou uvedeny v přiložených souborech, které jsou k dispozici online.

Description (English):

A Package for calculating elastic tensors of cubic structure by using second-order derivative with Wien2k code, this Package gives you the accurate values of the elastic constants of the cubic system. Results obtained by using this package are in very good agreement with the measured once. More details are described in the files attached to the package which are available online.

Installation:

1_ Copy “cubic-elastic.tar.gz” file in your computer. Then do the following;

tar –zxvf cubic-elastic.tar.gz

cd cubic-elastic

2_ Run **buildCIRelast_lapw**

This program helps you to provide "Makefile" and then compile cubic-elastic. Then define Environment Variable ELASTC_PATH and add it at the end of **.bashrc** file.

Requirements: Operation system Linux, Unix and WIEN2K code

Testing: the installation of software include some testing data

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