Equation of state and phase diagram of quartz ALEXANDER
PETROVTSEV, VLADIMIR DREMOV, VENER VILDANOV, MIKHAIL GOR-
SHKOV, VLADIMIR ZAHIKIN, YURII ZHUGIN, RFNC-VNIITF — On the basis
of the latest experimental data and ab-initio calculations the multi-phase equation
of state of quartz has been constructed. Quartz is a basic rock forming mineral.
This fact initiated a comprehensive investigation into its thermodynamic, mechan-
ical and shock-wave properties. Quartz has complicated phase diagram and one of
the very interesting problems having fundamental character is the study of the poly-
morphous and phase transformations in quartz at high pressures and temperatures
realizing when dynamic loading. Numerical modeling of these processes requires
multi-phase equation of state. Here we present such an equation of state including
a-quartz, stishovite and liquid quartz. Calculations carried out with the equation of
state are in good agreement with the experimental data on static and shock com-
pression of solid and porous quartz including the temperature measurements along
Hugoniots. On the basis of an analysis of the calculated phase diagram and porous
quartz Hugoniots the conclusions about what phase the legs of the experimental
Hugoniots belong to have been done.

Dean Preston
LANL

Date submitted: 12 Mar 2005   Electronic form version 1.4