RDF (X-RAY) ANALYSIS OF TIRAP COAL

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Abstract

XRD pattern of Tirap coal shows that it is amorphous in nature and its RDF study indicates that the coal is lignite in type. There is no evidence of graphite like structure. The first significant maximum in the RDF curve of the coal is found to be at r = 0.17 nm which relates to the C-C aliphatic bond length. The second maximum appears at r = 0.27 nm which relates to the distance between carbon atoms of aliphatic chains that are located across one carbon atom. Further, the maximum in the RDF curve is at r = 0.36 nm, which may be related to the distance between carbon atoms of aliphatic chain located across two carbon atoms. The g(r) curve of the coal clearly shows quite regular molecular packets.

Introduction

Coal is one of the most abundant energy resources and has the capability to meet future energy needs with high reliability. It is heterogeneous both macroscopically and microscopically. Although, coal has been utilized for several years the exact chemical nature of its structures are still not fully known. Coals of different chemical composition and therefore different structures, even within a certain age group (or rank) of coal such as lignite or bituminous coals, the structure may vary depending on the environment in which a particular coal was formed. Thus the concept of the coal structure is difficult to define, as the macromolecules of coal are not composed of repeating non-organic units.

The basic diffraction studies on coal structure were carried out many years ago [1-13]. Thus the studies indicate that the typical carbon content in coal is arranged in a macromolecular structure of condensed aromatic rings that form layer units, with bridges or "cross-links" formed by aliphatic and/ or other ethers conferring them a certain structure order [14-16].

Tirap coals have been classified as sub-bituminous on the basis of studies of the chemical composition and physical characteristics. The present work is concerned with the radial distribution function of atoms (RDFA) study of this coal.

Materials and Method

Experimental

Coal samples obtained from the Coal Chemistry Division of North East Institute of Science and Technology, Jorhat, were collected from Tirap coal (60' depth) mines of Makum coalfield. The samples were grounded < 150 microns before use. The X-ray diffractograms were obtained by using computer controlled X-ray diffractometer: Type JDX-11P3A, JEOL, JAPAN, attached with pulse height analyzer and scintillation counter with scientillator NaI single crystal. Measuring condition Mode: Voltage: 30 kV Start angle: 2.00, Target; Cu (Fe filtered), Current: 10 mA , Stop angle: 110,. The RDF calculation was carried out following a procedure given by Klug & Alexander [17]. *Corresponding author, Contact no. 09435489164

Theory

The radial distribution function (RDF) $4\pi r^2 \rho(r)$ and the pair distribution function $g(r) = 4\pi r\{\rho(r) - \rho_0\}$ for a substance consisting of one kind of atom are computed by the following relationships [17]: